

16 JUN 1998

09/091300

TRANSMITTAL LETTER TO THE UNITED STATES

ATTORNEY'S DOCKET NUMBER 47679

DESIGNATED/ELECTED OFFICE (DO/EO/US)
CONCERNING A FILING UNDER 35 U.S.C. 371

U.S. APPLICATION NO. (If known, see 37 CFR 1.5)

INTERNATIONAL APPLICATION NO.
PCT/EP 98/00069

INTERNATIONAL FILING DATE
8 January 1998

PRIORITY DATE CLAIMED
17 January 1997

TITLE OF INVENTION: 3-HETEROCYCLYL-SUBSTITUTED BENZOYL DERIVATIVES

APPLICANT(S) FOR DO/EO/US Wolfgang von DEYN, Regina Luise HILL, Uwe KARDORFF, Ernst BAUMANN, Stefan ENGEL,
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Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information:

1. /X/ This is a FIRST submission of items concerning a filing under 35 U.S.C. 371.
 2. / / This is a SECOND or SUBSEQUENT submission of items concerning a filing under 35 U.S.C. 371.
 3. /X/ This express request to begin national examination procedures (35 U.S.C. 371(f)) at any time rather than delay examination until the expiration of the applicable time limit set in 35 U.S.C. 371(b) and PCT Articles 22 and 39(1).
 4. /x / A proper Demand for International Preliminary Examination was made by the 19th month from the earliest claimed priority date.
 5. / / A copy of the International Application as filed (35 U.S.C. 371(c)(2)).
 - a. / / is transmitted herewith (required only if not transmitted by the International Bureau).
 - b. / / has been transmitted by the International Bureau.
 - c. / / is not required, as the application was filed in the United States Receiving Office (RO/USO).
 6. /X/ A translation of the International Application into English (35 U.S.C. 371(c)(2)).
 7. / / Amendments to the claims of the International Application under PCT Article 19 (35 U.S.C. 371(c)(3)).
 - a. / / are transmitted herewith (required only if not transmitted by the International Bureau).
 - b. / / have been transmitted by the International Bureau.
 - c. / / have not been made; however, the time limit for making such amendments has NOT expired.
 - d. / / have not been made and will not be made.
 8. / / A translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371(c)(3)).
 9. /X/ An oath or declaration of the inventor(s) (35 U.S.C. 171(c)(4)).
 10. / / A translation of the annexes to the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371(c)(5)).
- Items 11. to 16. below concern other document(s) or information included:
11. / / An Information Disclosure Statement under 37 CFR 1.97 and 1.98.
 12. /X/ An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 and 3.31 is included.
 13. /X/ A FIRST preliminary amendment.
/ / A SECOND or SUBSEQUENT preliminary amendment.
 14. / / A substitute specification.
 15. / / A change of power of attorney and/or address letter.
 16. /X/ Other items or information.
International Search Report
International Preliminary Examination Report

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U.S. Appln. No. (If Known) INTERNATIONAL APPLN. NO. ATTORNEY'S DOCKET NO.
PCT/EP 98/00069 47679

17. /X/ The following fees are submitted CALCULATIONS PTO USE ONLY
BASIC NATIONAL FEE (37 CFR 1.492(a)(1)-(5)):
Search Report has been prepared by the
EPO or JPO.....\$930.00 930.00

International preliminary examination fee paid to USPTO
(37 CFR 1.482).....\$750.00

No international preliminary examination fee paid to
USPTO (37 CFR 1.482) but international search fee paid
to USPTO (37 CFR 1.445(a)(2)).....\$700.00

Neither international preliminary examination fee
(37 CFR 1.482) nor international search fee
(37 CFR 1.445(a)(2)) paid to USPTO\$1,070.00

International preliminary examination fee paid to
USPTO (37 CFR 1.482) and all claims satisfied pro
-visions of PCT Article 33(2)-(4).....\$98.00

ENTER APPROPRIATE BASIC FEE AMOUNT = \$ 930.00

Surcharge of \$130.00 for furnishing the oath or declaration
later than / / 20 / 30 months from the earliest
claimed priority date (37 CFR 1.492(e)).

Claims	Number Filed	Number Extra	Rate
Total Claims	24 -20	4	X\$22. 88.00
Indep. Claims	5 -3	2	X\$82. 164.00
Multiple dependent claim(s) (if applicable)			+270.
TOTAL OF ABOVE CALCULATION			= 1,182.00

Reduction of 1/2 for filing by small entity, if applicable.
Verified Small Entity statement must also be filed
(Note 37 CFR 1.9, 1.27, 1.28).

SUBTOTAL = 1,182.00

Processing fee of \$130. for furnishing the English
translation later than / / 20 / 30 months from the
earliest claimed priority date (37 CFR 1.492(f)). +

TOTAL NATIONAL FEE = 1,182.00

Fee for recording the enclosed assignment (37 CFR 1.21(h)).
The assignment must be accompanied by an appropriate cover
sheet (37 CFR 3.28, 3.31) \$40.00 per property = 40.00

TOTAL FEES ENCLOSED = \$ 1,222.00

Amount to be

refunded: \$

Charged \$

a./X/ A check in the amount of \$1,222. to cover the above fees is enclosed.

b./ / Please charge my Deposit Account No. _____ in the amount of \$ _____ to cover the above
fees. A duplicate copy of this sheet is enclosed.

c./X/ The Commissioner is hereby authorized to charge any additional fees which may be required, or credit
any overpayment to Deposit Account No. 11-0345. A duplicate copy of this sheet is enclosed.

NOTE: Where an appropriate time limit under 37 CFR 1.494 or 1.495 has not been met, a petition to revive (37
CFR 1.137(a) or (b) must be filed and granted to restore the application to pending status.

SEND ALL CORRESPONDENCE TO:

KEIL & WEINKAUF
1101 Connecticut Ave., N.W.
Washington, D. C. 20036

Herbert B. Keil

NAME

18,967

Registration No.

SIGNATURE

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re the Application of)
von DEYN et al.)
) BOX PCT
International Application)
PCT/EP 98/00069)
)
Filed: January 8, 1997)
)
For: 3-HETEROCYCLYL-SUBSTITUTED BENZOYL DERIVATIVES

PRELIMINARY AMENDMENT

Honorable Commissioner of
Patents and Trademarks
Washington, D.C. 20231

Sir:

Prior to U.S. examination, kindly amend the above-identified
application as follows:

IN THE CLAIMS

Claim 3, line 2, delete "or 2".

Claim 4, line 2, delete "any of claims 1 to 3" and insert
--claim 1--.

Claim 5, line 2, delete "any of claims 1 to 4" and insert
--claim 1--.

Claim 6 line 2, delete "any of claims 1 to 4" and insert
--claim 1--.

Claim 7, line 2, delete "any of claims 1 to 4 or 6" and
insert --claim 1--.

Claim 8, line 2, delete "any of claims 1 to 4 or 6 or 7" and
insert --claim 1--.

Claim 9, line 2, delete "any of claims 1 to 4 or 6 to 8" and
insert --claim 1--.

Claim 10, line 2, delete "any of claims 1 to 4 or 6 or 7" and
insert --claim 1--.

Claim 11, line 2, delete "any of claims 1 to 4 or 6 or 7 or
10" and insert --claim 1--.

Claim 14, line 2, delete "any of claims 1 to 4 or 6" and
insert --claim 1--.

Claim 15, line 2, delete "any of claims 1 to 4 or 6 or 14"
and insert --claim 1--.

Claim 16, line 2, delete "any of claims 1 to 4 or 6 or 14"
and insert --claim 1--.

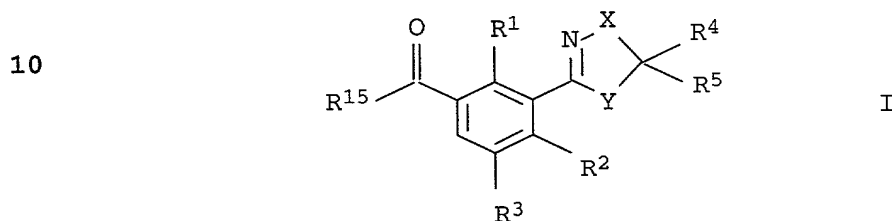
Claim 19, line 3, delete "under claims 2 to 16" and insert
--in claim 2--.

Claim 20, line 2, delete "either of claims 18 or 19" and
insert --claim 18--.

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3-Heterocyclyl-substituted benzoyl derivatives

5 The present invention relates to 3-heterocyclyl-substituted
benzoyl derivatives of the formula I



where the variables have the following meanings:

20 R^1, R^2 are hydrogen, nitro, halogen, cyano, C_1 - C_6 -alkyl, C_1 - C_6 -haloalkyl, C_1 - C_6 -alkoxy, C_1 - C_6 -haloalkoxy, C_1 - C_6 -alkylthio, C_1 - C_6 -haloalkylthio, C_1 - C_6 -alkylsulfinyl, C_1 - C_6 -haloalkylsulfinyl, C_1 - C_6 -alkylsulfonyl or C_1 - C_6 -haloalkylsulfonyl;

²⁵ R³ is hydrogen, halogen or C₁-C₆-alkyl;

R⁴, R⁵ are hydrogen, halogen, cyano, nitro, C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, di(C₁-C₄-alkoxy)-C₁-C₄-alkyl, di(C₁-C₄-alkyl)-amino-C₁-C₄-alkyl, [2,2-di(C₁-C₄-alkyl)-1-hydrazino]-C₁-C₄-alkyl, C₁-C₆-alkyliminoxy-C₁-C₄-alkyl, C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl, C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy, hydroxyl, C₁-C₄-alkylcarbonyloxy, C₁-C₄-alkylthio, C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be fully or partially halogenated and/or to have attached to them one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

45 or

2

R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

5

or

R⁴ and R⁵ together with the corresponding carbon form a carbonyl or thiocarbonyl group;

10

R⁶ is hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy, C₃-C₆-alkenyloxy, C₃-C₆-alkynyloxy or NR⁷R⁸;

15

R⁷ is hydrogen or C₁-C₄-alkyl;

R⁸ is C₁-C₄-alkyl;

20

X is O, S, NR⁹, CO or CR¹⁰R¹¹;

Y is O, S, NR¹², CO or CR¹³R¹⁴;

25

R⁹, R¹² are hydrogen or C₁-C₄-alkyl;

R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or CONR⁷R⁸;

30

or

R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

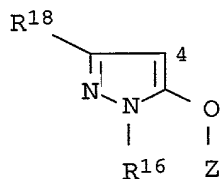
35

R¹⁵ is a pyrazole of the formula II which is linked in the 4-position

45

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3



II

where

R¹⁶ is C₁-C₆-alkyl;

Z is H or SO₂R¹⁷;

R¹⁷ is C₁-C₄-alkyl, C₁-C₄-haloalkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups:
nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

R¹⁸ is hydrogen or C₁-C₆-alkyl;

where X and Y are not simultaneously oxygen or sulfur;

with the exception of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-ethyl-5-hydroxy-1H-pyrazole, 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole, 4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole, 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and 4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;

or the agriculturally useful salts thereof.

The invention furthermore relates to processes and intermediates for the preparation of compounds of the formula I, to compositions comprising them, and to the use of these derivatives or compositions comprising them for the control of harmful plants.

Pyrazol-4-yl-benzoyl derivatives have been disclosed in the literature, for example in WO 96/26206.

However, the herbicidal properties of the compounds which have
5 been known to date and their compatibility properties regarding crop plants are only moderately satisfactory.

It is an object of the present invention to provide novel, in
10 particular herbicidally active, compounds which have improved properties.

We have found that this object is achieved by the 3-hetero-
cyclyl-substituted benzoyl derivatives of the formula I and by
15 their herbicidal activity.

We have furthermore found herbicidal compositions which comprise
the compounds I and which have a very good herbicidal activity.
Moreover, we have found processes for the preparation of these
20 compositions and methods of controlling undesirable vegetation using the compounds I.

Depending on the substitution pattern, the compounds of the
formula I can contain one or more chiral centers, in which case
25 they exist as enantiomer or diastereomer mixtures. The present invention relates to the pure enantiomers or diastereomers and to the mixtures thereof.

The compounds of the formula I may also exist in the form of
30 their agriculturally useful salts, the type of salt generally being of no importance. In general, suitable salts are the salts of those cations or the acid addition salts of those acids whose cations, or anions, respectively, do not adversely affect the
35 herbicidal activity of the compounds I.

Suitable cations are, in particular, ions of the alkali metals, preferably lithium, sodium and potassium, of the alkaline earth metals, preferably calcium and magnesium, and of the transition
40 metals, preferably manganese, copper, zinc and iron, and also ammonium, it being possible in this case, if desired, for one to four hydrogen atoms to be replaced by C₁-C₄-alkyl, hydroxy-C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, hydroxy-C₁-C₄-alkoxy-C₁-C₄-alkyl, phenyl or benzyl, preferably
45 ammonium, dimethylammonium, diisopropylammonium, tetramethylammonium, tetrabutylammonium, 2-(2-hydroxyeth-1-oxy)eth-1-ylammonium,

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di(2-hydroxyeth-1-yl)ammonium, trimethylbenzylammonium, in addition phosphonium ions, sulfonium ions, preferably tri(C₁-C₄-alkyl)sulfonium and sulfoxonium ions, preferably tri(C₁-C₄-alkyl)sulfoxonium.

5

Anions of useful acid addition salts are mainly chloride, bromide, fluoride, hydrogen sulfate, sulfate, dihydrogen phosphate, hydrogen phosphate, nitrate, hydrogen carbonate, carbonate, hexafluorosilicate, hexafluorophosphate, benzoate, and
 10 the anions of C₁-C₄-alkanoic acids, preferably formate, acetate, propionate and butyrate.

The organic moieties mentioned for the substituents R¹-R¹⁸ or as
 15 radicals on phenyl rings are collective terms for individual enumerations of the individual group members. All hydrocarbon chains, ie. all alkyl, haloalkyl, cyanoalkyl, alkoxy, haloalkoxy, alkyliminooxy, alkylcarbonyloxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl,
 20 haloalkylsulfonyl, alkoxycarbonyl, haloalkoxycarbonyl, alkenyloxy, alkynyloxy, dialkylamino, dialkylhydrazino, alkoxyalkyl, hydroxyalkoxyalkyl, dialkoxyalkyl, alkylthioalkyl, dialkylaminoalkyl, dialkylhydrazinoalkyl, alkyliminooxyalkyl, alkoxycarbonylalkyl and alkoxyalkoxy moieties, can be
 25 straight-chain or branched. Unless otherwise specified, halogenated substituents preferably have attached to them one to five identical or different halogen atoms. The meaning of halogen is in each case fluorine, chlorine, bromine or iodine.

30 Other examples of meanings are:

- C₁-C₄-alkyl and the alkyl moieties of di-(C₁-C₄-alkoxy)-C₁-C₄-alkyl, [2,2-di(C₁-C₄-alkyl)-1-hydrazino]-C₁-C₄-alkyl, C₁-C₆-alkyliminooxy-C₁-C₄-alkyl, hydroxy-C₁-C₄-alkoxy-C₁-C₄-alkyl and C₁-C₄-alkylcarbonyloxy: for example methyl,
 35 ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl and 1,1-dimethylethyl;
- C₁-C₆-alkyl: C₁-C₄-alkyl as mentioned above and, for example,
 40 pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 2,2-dimethylpropyl, 1-ethylpropyl, hexyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 1-methylpentyl, 2-methylpentyl, 3-methylpentyl, 4-methylpentyl, 1,1-dimethylbutyl, 1,2-dimethylbutyl, 1,3-dimethylbutyl, 2,2-dimethylbutyl,
 45 2,3-dimethylbutyl, 3,3-dimethylbutyl, 1-ethylbutyl,

2-ethylbutyl, 1,1,2-trimethylpropyl, 1-ethyl-1-methylpropyl and 1-ethyl-3-methylpropyl;

- 5 - C₁-C₄-haloalkyl: a C₁-C₄-alkyl radical as mentioned above which is partially or fully substituted by fluorine, chlorine, bromine and/or iodine, for example chloromethyl, dichloromethyl, trichloromethyl, fluoromethyl, difluoromethyl, trifluoromethyl, chlorofluoromethyl, dichlorofluoromethyl, chlorodifluoromethyl, 2-fluoroethyl, 10 2-chloroethyl, 2-bromoethyl, 2-iodoethyl, 2,2-difluoroethyl, 2,2,2-trifluoroethyl, 2-chloro-2-fluoroethyl, 2-chloro-2,2-difluoroethyl, 2,2-dichloro-2-fluoroethyl, 2,2,2-trichloroethyl, pentafluoroethyl, 2-fluoropropyl, 3-fluoropropyl, 2,2-difluoropropyl, 2,3-difluoropropyl, 15 2-chloropropyl, 3-chloropropyl, 2,3-dichloropropyl, 2-bromopropyl, 3-bromopropyl, 3,3,3-trifluoropropyl, 3,3,3-trichloropropyl, 2,2,3,3,3-pentafluoropropyl, heptafluoropropyl, 1-(fluoromethyl)-2-fluoroethyl, 1-(chloromethyl)-2-chloroethyl, 1-(bromomethyl)-2-bromoethyl, 20 4-fluorobutyl, 4-chlorobutyl, 4-bromobutyl and nonafluorobutyl;
- C₁-C₆-haloalkyl: C₁-C₄-haloalkyl as mentioned above and, for example, 5-fluoropentyl, 5-chloropentyl, 5-bromopentyl, 25 5-iodopentyl, undecafluoropentyl, 6-fluorohexyl, 6-chlorohexyl, 6-bromohexyl, 6-iodohexyl and dodecafluorohexyl;
- 30 - C₁-C₄-cyanoalkyl: for example cyanomethyl, 1-cyanoeth-1-yl, 2-cyanoeth-1-yl, 1-cyanoprop-1-yl, 2-cyanoprop-1-yl, 3-cyanoprop-1-yl, 1-cyanoprop-2-yl, 2-cyanoprop-2-yl, 1-cyanobut-1-yl, 2-cyanobut-1-yl, 3-cyanobut-1-yl, 4-cyanobut-1-yl, 1-cyanobut-2-yl, 2-cyanobut-2-yl, 35 1-cyanobut-3-yl, 2-cyanobut-3-yl, 1-cyano-2-methylprop-3-yl, 2-cyano-2-methylprop-3-yl, 3-cyano-2-methylprop-3-yl and 2-cyanomethylprop-2-yl;
- C₁-C₄-alkoxy and the alkoxy moieties of di-(C₁-C₄-alkoxy)- 40 C₁-C₄-alkyl and hydroxy-C₁-C₄-alkoxy-C₁-C₄-alkyl: for example methoxy, ethoxy, propoxy, 1-methylethoxy, butoxy, 1-methylpropoxy, 2-methylpropoxy and 1,1-dimethylethoxy;
- C₁-C₆-alkoxy: C₁-C₄-alkoxy as mentioned above and, for 45 example, pentoxy, 1-methylbutoxy, 2-methylbutoxy, 3-methoxylbutoxy, 1,1-dimethylpropoxy, 1,2-dimethylpropoxy, 2,2-dimethylpropoxy, 1-ethylpropoxy, hexoxy, 1-methylpentoxy,

- 2-methylpentoxy, 3-methylpentoxy, 4-methylpentoxy,
1,1-dimethylbutoxy, 1,2-dimethylbutoxy, 1,3-dimethylbutoxy,
2,2-dimethylbutoxy, 2,3-dimethylbutoxy, 3,3-dimethylbutoxy,
1-ethylbutoxy, 2-ethylbutoxy, 1,1,2-trimethylpropoxy,
5 1,2,2-trimethylpropoxy, 1-ethyl-1-methylpropoxy and
1-ethyl-2-methylpropoxy;
- C₁-C₄-haloalkoxy: a C₁-C₄-alkoxy radical as mentioned above
which is partially or fully substituted by fluorine,
10 chlorine, bromine and/or iodine, for example fluoromethoxy,
difluoromethoxy, trifluoromethoxy, chlorodifluoromethoxy,
bromodifluoromethoxy, 2-fluoroethoxy, 2-chloroethoxy,
2-bromomethoxy, 2-iodoethoxy, 2,2-difluoroethoxy,
2,2,2-trifluoroethoxy, 2-chloro-2-fluoroethoxy,
15 2-chloro-2,2-difluoroethoxy, 2,2-dichloro-2-fluoroethoxy,
2,2,2-trichloroethoxy, pentafluoroethoxy, 2-fluoropropoxy,
3-fluoropropoxy, 2-chloropropoxy, 3-chloropropoxy,
2-bromopropoxy, 3-bromopropoxy, 2,2-difluoropropoxy,
2,3-difluoropropoxy, 2,3-dichloropropoxy,
20 3,3,3-trifluoropropoxy, 3,3,3-trichloropropoxy,
2,2,3,3,3-pentafluoropropoxy, heptafluoropropoxy,
1-(fluoromethyl)-2-fluoroethoxy,
1-(chloromethyl)-2-chloroethoxy,
1-(bromomethyl)-2-bromoethoxy, 4-fluorobutoxy,
25 4-chlorobutoxy, 4-bromobutoxy and nonafluorobutoxy;
- C₁-C₆-haloalkoxy: C₁-C₄-haloalkoxy as mentioned above and, for
example, 5-fluoropentoxy, 5-chloropentoxy, 5-bromopentoxy,
5-iodopentoxy, undecafluoropentoxy, 6-fluorohexoxy,
30 6-chlorohexoxy, 6-bromohexoxy, 6-iodohexoxy and
dodecafluorohexoxy;
- C₁-C₆-alkyliminoxy and the C₁-C₆-alkyliminoxy moieties of
35 C₁-C₆-alkyliminoxy-C₁-C₄-alkyl: for example methyliminoxy,
ethyliminoxy, 1-propyliminoxy, 2-propyliminoxy,
1-butyliminoxy, 2-butyliminoxy, 2-methylprop-1-yliminoxy,
1-pentyliminoxy, 2-pentyliminoxy, 3-pentyliminoxy,
3-methylbut-2-yliminoxy, 2-methylbut-1-yliminoxy,
40 3-methylbut-1-yliminoxy, 1-hexyliminoxy, 2-Hexyliminoxy,
3-hexyliminoxy, 2-methylpent-1-yliminoxy,
3-methylpent-1-yliminoxy, 4-methylpent-1-yliminoxy,
2-ethylbut-1-yliminoxy, 3-ethylbut-1-yliminoxy,
2,3-dimethylbut-1-yliminoxy, 3-methylpent-2-yliminoxy,
45 4-methylpent-2-yliminoxy and 3,3-dimethylbut-2-yliminoxy;

- C₁-C₄-alkylthio: for example methylthio, ethylthio, propylthio, 1-methylethylthio, butylthio, 1-methylpropylthio, 2-methylpropylthio and 1,1-dimethylethylthio;
- 5 - C₁-C₆-alkylthio: C₁-C₄-alkylthio as mentioned above and, for example, pentylthio, 1-methylbutylthio, 2-methylbutylthio, 3-methylbutylthio, 2,2-dimethylpropylthio, 1-ethylpropylthio, hexylthio, 1,1-dimethylpropylthio, 1,2-dimethylpropylthio, 1-methylpentylthio, 2-methylpentylthio, 3-methylpentylthio, 4-methylpentylthio, 1,1-dimethylbutylthio, 1,2-dimethylbutylthio, 1,3-dimethylbutylthio, 2,2-dimethylbutylthio, 2,3-dimethylbutylthio, 3,3-dimethylbutylthio, 1-ethylbutylthio, 2-ethylbutylthio, 1,1,2-trimethylpropylthio, 1,2,2-trimethylpropylthio, 1-ethyl-1-methylpropylthio and 1-ethyl-2-methylpropylthio;
- 10
- 15
- C₁-C₄-haloalkylthio: a C₁-C₄-alkylthio radical as mentioned above, which is partially or fully substituted by fluorine, chlorine, bromine and/or iodine, for example
- 20 fluoromethylthio, difluoromethylthio, trifluoromethylthio, chlorodifluoromethylthio, bromodifluoromethylthio, 2-fluoroethylthio, 2-chloroethylthio, 2-bromoethylthio, 2-iodoethylthio, 2,2-difluoroethylthio, 2,2,2-trifluoroethylthio, 2,2,2-trichloroethylthio, 2-chloro-2-fluoroethylthio, 2-chloro-2,2-difluoroethylthio, 2,2-dichloro-2-fluoroethylthio, pentafluoroethylthio, 2-fluoropropylthio, 3-fluoropropylthio, 2-chloropropylthio, 3-chloropropylthio, 2-bromopropylthio, 3-bromopropylthio, 2,2-difluoropropylthio, 2,3-difluoropropylthio, 2,3-dichloropropylthio, 3,3,3-trifluoropropylthio, 3,3,3-trichloropropylthio, 2,2,3,3,3-pentafluoropropylthio, heptafluoropropylthio, 1-(fluoromethyl)-2-fluoroethylthio, 1-(chloromethyl)-2-chloroethylthio, 1-(bromomethyl)-2-bromoethylthio, 4-fluorobutylthio, 4-chlorobutylthio, 4-bromobutylthio and nonafluorobutylthio;
- 25
- 30
- 35
- C₁-C₆-haloalkylthio: C₁-C₄-haloalkylthio as mentioned above and, for example, 5-fluoropentylthio, 5-chloropentylthio, 5-bromopentylthio, 5-iodopentylthio, undecafluoropentylthio, 6-fluorohexylthio, 6-chlorohexylthio, 6-bromohexylthio, 6-iodohexylthio and dodecafluorohexylthio;
- 40
- C₁-C₆-alkylsulfinyl (C₁-C₆-alkyl-S(=O)-): for example methylsulfinyl, ethylsulfinyl, propylsulfinyl, 1-methylethylsulfinyl, butylsulfinyl, 1-methylpropylsulfinyl, 2-methylpropylsulfinyl, 1,1-dimethylethylsulfinyl,
- 45

- pentylsulfinyl, 1-methylbutylsulfinyl, 2-methylbutylsulfinyl,
 3-methylbutylsulfinyl, 2,2-dimethylpropylsulfinyl,
 1-ethylpropylsulfinyl, 1,1-dimethylpropylsulfinyl,
 1,2-dimethylpropylsulfinyl, hexylsulfinyl,
 5 1-methylpentylsulfinyl, 2-methylpentylsulfinyl,
 3-methylpentylsulfinyl, 4-methylpentylsulfinyl,
 1,1-dimethylbutylsulfinyl, 1,2-dimethylbutylsulfinyl,
 1,3-dimethylbutylsulfinyl, 2,2-dimethylbutylsulfinyl,
 2,3-dimethylbutylsulfinyl, 3,3-dimethylbutylsulfinyl,
 10 1-ethylbutylsulfinyl, 2-ethylbutylsulfinyl,
 1,1,2-trimethylpropylsulfinyl, 1,2,2-trimethylpropylsulfinyl,
 1-ethyl-1-methylpropylsulfinyl and
 1-ethyl-2-methylpropylsulfinyl;
- 15 - C₁-C₆-haloalkylsulfinyl: a C₁-C₆-alkylsulfinyl radical as
 mentioned above which is partially or fully substituted by
 fluorine, chlorine, bromine and/or iodine, for example
 fluoromethylsulfinyl, difluoromethylsulfinyl,
 20 trifluoromethylsulfinyl, chlorodifluoromethylsulfinyl,
 bromodifluoromethylsulfinyl, 2-fluoroethylsulfinyl,
 2-chloroethylsulfinyl, 2-bromoethylsulfinyl,
 2-iodoethylsulfinyl, 2,2-difluoroethylsulfinyl,
 2,2,2-trifluoroethylsulfinyl, 2,2,2-trichloroethylsulfinyl,
 2-chloro-2-fluoroethylsulfinyl,
 25 2-chloro-2,2-difluoroethylsulfinyl,
 2,2-dichloro-2-fluoroethylsulfinyl, pentafluoroethylsulfinyl,
 2-fluoropropylsulfinyl, 3-fluoropropylsulfinyl,
 2-chloropropylsulfinyl, 3-chloropropylsulfinyl,
 2-bromopropylsulfinyl, 3-bromopropylsulfinyl,
 30 2,2-difluoropropylsulfinyl, 2,3-difluoropropylsulfinyl,
 2,3-dichloropropylsulfinyl, 3,3,3-trifluoropropylsulfinyl,
 3,3,3-trichloropropylsulfinyl,
 2,2,3,3,3-pentafluoropropylsulfinyl,
 heptafluoropropylsulfinyl,
 35 1-(fluoromethyl)-2-fluoroethylsulfinyl,
 1-(chloromethyl)-2-chloroethylsulfinyl,
 1-(bromomethyl)-2-bromoethylsulfinyl, 4-fluorobutylsulfinyl,
 4-chlorobutylsulfinyl, 4-bromobutylsulfinyl,
 nonafluorobutylsulfinyl, 5-fluoropentylsulfinyl,
 40 5-chloropentylsulfinyl, 5-bromopentylsulfinyl,
 5-iodopentylsulfinyl, undecafluoropentylsulfinyl,
 6-fluorohexylsulfinyl, 6-chlorohexylsulfinyl,
 6-bromohexylsulfinyl, 6-iodohexylsulfinyl and
 dodecafluorohexylsulfinyl;
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- C₁-C₆-alkylsulfonyl (C₁-C₆-alkyl-S(=O)₂-): for example
 methylsulfonyl, ethylsulfonyl, propylsulfonyl,
 1-methylethylsulfonyl, butylsulfonyl, 1-methylpropylsulfonyl,
 2-methylpropylsulfonyl, 1,1-dimethylethylsulfonyl,
 5 pentylsulfonyl, 1-methylbutylsulfonyl, 2-methylbutylsulfonyl,
 3-methylbutylsulfonyl, 1,1-dimethylpropylsulfonyl,
 1,2-dimethylpropylsulfonyl, 2,2-dimethylpropylsulfonyl,
 1-ethylpropylsulfonyl, hexylsulfonyl, 1-methylpentylsulfonyl,
 2-methylpentylsulfonyl, 3-methylpentylsulfonyl,
 10 4-methylpentylsulfonyl, 1,1-dimethylbutylsulfonyl,
 1,2-dimethylbutylsulfonyl, 1,3-dimethylbutylsulfonyl,
 2,2-dimethylbutylsulfonyl, 2,3-dimethylbutylsulfonyl,
 3,3-dimethylbutylsulfonyl, 1-ethylbutylsulfonyl,
 2-ethylbutylsulfonyl, 1,1,2-trimethylpropylsulfonyl,
 15 1,2,2-trimethylpropylsulfonyl, 1-ethyl-1-methylpropylsulfonyl
 and 1-ethyl-2-methylpropylsulfonyl;

- C₁-C₆-haloalkylsulfonyl: a C₁-C₆-alkylsulfonyl radical as
 mentioned above which is partially or fully substituted by
 20 fluorine, chlorine, bromine and/or iodine, for example
 fluoromethylsulfonyl, difluoromethylsulfonyl,
 trifluoromethylsulfonyl, chlorodifluoromethylsulfonyl,
 bromodifluoromethylsulfonyl, 2-fluoroethylsulfonyl,
 2-chloroethylsulfonyl, 2-bromoethylsulfonyl,
 25 2-iodoethylsulfonyl, 2,2-difluoroethylsulfonyl,
 2,2,2-trifluoroethylsulfonyl, 2-chloro-2-fluoroethylsulfonyl,
 2-chloro-2,2-difluoroethylsulfonyl,
 2,2-dichloro-2-fluoroethylsulfonyl,
 2,2,2-trichloroethylsulfonyl, pentafluoroethylsulfonyl,
 30 2-fluoropropylsulfonyl, 3-fluoropropylsulfonyl,
 2-chloropropylsulfonyl, 3-chloropropylsulfonyl,
 2-bromopropylsulfonyl, 3-bromopropylsulfonyl,
 2,2-difluoropropylsulfonyl, 2,3-difluoropropylsulfonyl,
 2,3-dichloropropylsulfonyl, 3,3,3-trifluoropropylsulfonyl,
 35 3,3,3-trichloropropylsulfonyl,
 2,2,3,3,3-pentafluoropropylsulfonyl,
 heptafluoropropylsulfonyl,
 1-(fluoromethyl)-2-fluoroethylsulfonyl, 1-(chloromethyl)-2-
 chloroethylsulfonyl, 1-(bromomethyl)-2-bromoethylsulfonyl,
 40 4-fluorobutylsulfonyl, 4-chlorobutylsulfonyl,
 4-bromobutylsulfonyl, nonafluorobutylsulfonyl,
 5-fluoropentylsulfonyl, 5-chloropentylsulfonyl,
 5-bromopentylsulfonyl, 5-iodopentylsulfonyl,
 6-fluorohexylsulfonyl, 6-bromohexylsulfonyl,
 45 6-iodohexylsulfonyl and dodecafluorohexylsulfonyl;

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- C₁-C₄-alkoxycarbonyl: for example methoxycarbonyl, ethoxycarbonyl, propoxycarbonyl, 1-methylethoxycarbonyl, butoxycarbonyl, 1-methylpropoxycarbonyl, 2-methylpropoxycarbonyl and 1,1-dimethoxycarbonyl;
- 5
- C₁-C₄-haloalkoxycarbonyl: a C₁-C₄-alkoxycarbonyl as mentioned above which is partially or fully substituted by fluorine, chlorine, bromine and/or iodine, for example
- 10
- fluoromethoxycarbonyl, difluoromethoxycarbonyl, trifluoromethoxycarbonyl, chlorodifluoromethoxycarbonyl, bromodifluoromethoxycarbonyl, 2-fluoroethoxycarbonyl, 2-chloroethoxycarbonyl, 2-bromoethoxycarbonyl, 2-iodoethoxycarbonyl, 2,2-difluoroethoxycarbonyl, 2,2,2-trifluoroethoxycarbonyl,
- 15
- 2-chloro-2-fluoroethoxycarbonyl, 2-chloro-2,2-difluoroethoxycarbonyl, 2,2-dichloro-2-fluoroethoxycarbonyl, 2,2,2-trichloroethoxycarbonyl, pentafluoroethoxycarbonyl, 2-fluoropropoxycarbonyl, 3-fluoropropoxycarbonyl,
- 20
- 2-chloropropoxycarbonyl, 3-chloropropoxycarbonyl, 2-bromopropoxycarbonyl, 3-bromopropoxycarbonyl, 2,2-difluoropropoxycarbonyl, 2,3-difluoropropoxycarbonyl, 2,3-dichloropropoxycarbonyl, 3,3,3-trifluoropropoxycarbonyl, 3,3,3-trichloropropoxycarbonyl,
- 25
- 2,2,3,3,3-pentafluoropropoxycarbonyl, heptafluoropropoxycarbonyl, 1-(fluoromethyl)-2-fluoroethoxycarbonyl, 1-(chloromethyl)-2-chloroethoxycarbonyl, 1-(bromomethyl)-2-bromoethoxycarbonyl,
- 30
- 4-fluorobutoxycarbonyl, 4-chlorobutoxycarbonyl, 4-bromobutoxycarbonyl and 4-iodobutoxycarbonyl;
-
- C₃-C₆-alkenyloxy: for example prop-1-en-1-yloxy, prop-2-en-1-yloxy, 1-methylethenyloxy, buten-1-yloxy,
- 35
- buten-2-yloxy, buten-3-yloxy, 1-methylprop-1-en-1-yloxy, 2-methylprop-1-en-1-yloxy, 1-methylprop-2-en-1-yloxy, 2-methylprop-2-en-1-yloxy, penten-1-yloxy, penten-2-yloxy, penten-3-yloxy, penten-4-yloxy, 1-methylbut-1-en-1-yloxy,
- 40
- 2-methylbut-1-en-1-yloxy, 3-methylbut-1-en-1-yloxy, 1-methylbut-2-en-1-yloxy, 2-methylbut-2-en-1-yloxy, 3-methylbut-2-en-1-yloxy, 1-methylbut-3-en-1-yloxy, 2-methylbut-3-en-1-yloxy, 3-methylbut-3-en-1-yloxy,
- 45
- 1,1-dimethylprop-2-en-1-yloxy, 1,2-dimethylprop-1-en-1-yloxy, 1,2-dimethylprop-2-en-1-yloxy, 1-ethylprop-1-en-2-yloxy, 1-ethylprop-2-en-1-yloxy, hex-1-en-1-yloxy, hex-2-en-1-yloxy, hex-3-en-1-yloxy, hex-4-en-1-yloxy, hex-5-en-1-yloxy, 1-methylpent-1-en-1-yloxy, 2-methylpent-1-en-1-yloxy,

- 3-methylpent-1-en-1-yloxy, 4-methylpent-1-en-1-yloxy,
 1-methylpent-2-en-1-yloxy, 2-methylpent-2-en-1-yloxy,
 3-methylpent-2-en-1-yloxy, 4-methylpent-2-en-1-yloxy,
 1-methylpent-3-en-1-yloxy, 2-methylpent-3-en-1-yloxy,
 5 3-methylpent-3-en-1-yloxy, 4-methylpent-3-en-1-yloxy,
 1-methylpent-4-en-1-yloxy, 2-methylpent-4-en-1-yloxy,
 3-methylpent-4-en-1-yloxy, 4-methylpent-4-en-1-yloxy,
 1,1-dimethylbut-2-en-1-yloxy, 1,1-dimethylbut-3-en-1-yloxy,
 1,2-dimethylbut-1-en-1-yloxy, 1,2-dimethylbut-2-en-1-yloxy,
 10 1,2-dimethylbut-3-en-1-yloxy, 1,3-dimethylbut-1-en-1-yloxy,
 1,3-dimethylbut-2-en-1-yloxy, 1,3-dimethylbut-3-en-1-yloxy,
 2,2-dimethylbut-3-en-1-yloxy, 2,3-dimethylbut-1-en-1-yloxy,
 2,3-dimethylbut-2-en-1-yloxy, 2,3-dimethylbut-3-en-1-yloxy,
 3,3-dimethylbut-1-en-1-yloxy, 3,3-dimethylbut-2-en-1-yloxy,
 15 1-ethylbut-1-en-1-yloxy, 1-ethylbut-2-en-1-yloxy,
 1-ethylbut-3-en-1-yloxy, 2-ethylbut-1-en-1-yloxy,
 2-ethylbut-2-en-1-yloxy, 2-ethylbut-3-en-1-yloxy,
 1,1,2-trimethylprop-2-en-1-yloxy,
 1-ethyl-1-methylprop-2-en-1-yloxy,
 20 1-ethyl-2-methylprop-1-en-1-yloxy and
 1-ethyl-2-methylprop-2-en-1-yloxy;
- C₃-C₆-alkynyloxy: for example prop-1-yn-1-yloxy,
 prop-2-yn-1-yloxy, but-1-yn-1-yloxy, but-1-yn-3-yloxy,
 25 but-1-yn-4-yloxy, but-2-yn-1-yloxy, pent-1-yn-1-yloxy,
 pent-1-yn-3-yloxy, pent-1-yn-4-yloxy, pent-1-yn-5-yloxy,
 pent-2-yn-1-yloxy, pent-2-yn-4-yloxy, pent-2-yn-5-yloxy,
 3-methylbut-1-yn-3-yloxy, 3-methylbut-1-yn-4-yloxy,
 hex-1-yn-1-yloxy, hex-1-yn-3-yloxy, hex-1-yn-4-yloxy,
 30 hex-1-yn-5-yloxy, hex-1-yn-6-yloxy, hex-2-yn-1-yloxy,
 hex-2-yn-4-yloxy, hex-2-yn-5-yloxy, hex-2-yn-6-yloxy,
 hex-3-yn-1-yloxy, hex-3-yn-2-yloxy,
 3-methylpent-1-yn-1-yloxy, 3-methylpent-1-yn-3-yloxy,
 3-methylpent-1-yn-4-yloxy, 3-methylpent-1-yn-5-yloxy,
 35 4-methylpent-1-yn-1-yloxy, 4-methylpent-2-yn-4-yloxy and
 4-methylpent-2-yn-5-yloxy;
- di(C₁-C₄-alkyl)amino: for example N,N-dimethylamino,
 N,N-diethylamino, N,N-dipropylamino,
 40 N,N-di(1-methylethyl)amino, N,N-dibutylamino,
 N,N-di(1-methylpropyl)amino, N,N-di(2-methylpropyl)amino,
 N,N-di(1,1-dimethylethyl)amino, N-ethyl-N-methylamino,
 N-methyl-N-propylamino, N-methyl-N-(1-methylethyl)amino,
 N-butyl-N-methylamino, N-methyl-N-(1-methylpropyl)amino,
 45 N-methyl-N-(2-methylpropyl)amino,
 N-(1,1-dimethylethyl)-N-methylamino, N-ethyl-N-propylamino,
 N-ethyl-N-(1-methylethyl)amino, N-butyl-N-ethylamino,

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- N-ethyl-N-(1-methylpropyl) amino,
 N-ethyl-N-(2-methylpropyl) amino,
 N-ethyl-N-(1,1-dimethylethyl) amino,
 N-(1-methylethyl)-N-propylamino, N-butyl-N-propylamino,
 5 N-(1-methylpropyl)-N-propylamino,
 N-(2-methylpropyl)-N-propylamino,
 N-(1,1-dimethylethyl)-N-propylamino,
 N-butyl-N-(1-methylethyl) amino,
 N-(1-methylethyl)-N-(1-methylpropyl) amino,
 10 N-(1-methylethyl)-N-(2-methylpropyl) amino,
 N-(1,1-dimethylethyl)-N-(1-methylethyl) amino,
 N-butyl-N-(1-methylpropyl) amino,
 N-butyl-N-(2-methylpropyl) amino,
 N-butyl-N-(1,1-dimethylethyl) amino,
 15 N-(1-methylpropyl)-N-(2-methylpropyl) amino,
 N-(1,1-dimethylethyl)-N-(1-methylpropyl) amino and
 N-(1,1-dimethylethyl)-N-(2-methylpropyl) amino;
- [2,2-di(C₁-C₄-alkyl)-1-hydrazino], and the dialkylhydrazino
 20 moieties of [2,2-di(C₁-C₄-alkyl)-1-hydrazino]-C₁-C₄-alkyl: for
 example 2,2-dimethylhydrazino-1, 2,2-diethylhydrazino-1,
 2,2-dipropylhydrazino-1, 2,2-di(1-methylethyl)-1-hydrazino,
 2,2-dibutylhydrazino-1, 2,2-di(1-methylpropyl)-1-hydrazino,
 2,2-di(2-methylpropyl)-1-hydrazino,
 25 2,2-di(1,1-dimethylethyl)-1-hydrazino,
 2-ethyl-2-methyl-1-hydrazino, 2-methyl-2-propyl-1-hydrazino,
 2-methyl-2-(1-methylethyl)-1-hydrazino,
 2-butyl-2-methyl-1-hydrazino,
 2-methyl-2-(1-methylpropyl)-1-hydrazino,
 30 2-methyl-2-(2-methylpropyl)-1-hydrazino,
 2-(1,1-dimethylethyl)-2-methyl-1-hydrazino,
 2-ethyl-2-propyl-1-hydrazino,
 2-ethyl-2-(1-methylethyl)-1-hydrazino,
 2-butyl-2-ethyl-1-hydrazino,
 35 2-ethyl-2-(1-methylpropyl)-1-hydrazino,
 2-ethyl-2-(2-methylpropyl)-1-hydrazino,
 2-ethyl-2-(1,1-dimethylethyl)-1-hydrazino,
 2-(1-methylethyl)-2-propyl-1-hydrazino,
 2-butyl-2-propyl-1-hydrazino,
 40 2-(1-methylpropyl)-2-propyl-1-hydrazino,
 2-(2-methylpropyl)-2-propyl-1-hydrazino,
 2-(1,1-dimethylethyl)-2-propyl-1-hydrazino,
 2-butyl-2-(1-methylethyl)-1-hydrazino,
 2-(1-methylethyl)-2-(1-methylpropyl)-1-hydrazino,
 45 2-(1-methylethyl)-2-(2-methylpropyl)-1-hydrazino,
 2-(1,1-dimethylethyl)-2-(1-methylethyl)-1-hydrazino,
 2-butyl-2-(1-methylpropyl)-1-hydrazino,

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- 2-butyl-2-(2-methylpropyl)-1-hydrazino,
 2-butyl-2-(1,1-dimethylethyl)-1-hydrazino,
 2-(1-methylpropyl)-2-(2-methylpropyl)-1-hydrazino,
 2-(1,1-dimethylethyl)-2-(1-methylpropyl)-1-hydrazino and
 5 2-(1,1-dimethylethyl)-2-(2-methylpropyl)-1-hydrazino;
- di(C₁-C₄-alkyl)amino-C₁-C₄-alkyl: C₁-C₄-alkyl which is substituted by di(C₁-C₄-alkyl)amino as mentioned above, for example N,N-dimethylaminomethyl, N,N-diethylaminomethyl,
 10 N,N-dipropylaminomethyl, N,N-di(1-methylethyl)aminomethyl, N,N-dibutylaminomethyl, N,N-di(1-methylpropyl)aminomethyl, N,N-di(2-methylpropyl)aminomethyl, N,N-di(1,1-dimethylethyl)aminomethyl, N-ethyl-N-methylaminomethyl, N-methyl-N-propylaminomethyl,
 15 N-methyl-N-(1-methylethyl)aminomethyl, N-butyl-N-methylaminomethyl, N-methyl-N-(1-methylpropyl)aminomethyl, N-methyl-N-(2-methylpropyl)aminomethyl, N-(1,1-dimethylethyl)-N-methylaminomethyl, N-ethyl-N-propylaminomethyl, N-ethyl-N-(1-methylethyl)aminomethyl, N-butyl-N-ethylaminomethyl, N-ethyl-N-(1-methylpropyl)aminomethyl, N-ethyl-N-(2-methylpropyl)aminomethyl, N-ethyl-N-(1,1-di-
 25 methylethyl)aminomethyl, N-(1-methylethyl)-N-propylaminomethyl, N-butyl-N-propylaminomethyl, N-(1-methylpropyl)-N-propylaminomethyl, N-(2-methylpropyl)-N-propylaminomethyl, N-(1,1-dimethylethyl)-N-propylaminomethyl, N-butyl-N-(1-methylethyl)aminomethyl, N-(1-methylethyl)-N-(1-methylpropyl)aminomethyl, N-(1-methylethyl)-N-(2-methylpropyl)aminomethyl, N-(1,1-dimethylethyl)-N-(1-methylethyl)aminomethyl, N-butyl-N-(1-methylpropyl)aminomethyl, N-butyl-N-(2-methylpropyl)aminomethyl, N-butyl-N-(1,1-dimethylethyl)aminomethyl, N-(1-methylpropyl)-N-(2-methylpropyl)aminomethyl, N-(1,1-dimethylethyl)-N-(1-methylpropyl)aminomethyl,
 40 N-(1,1-dimethylethyl)-N-(2-methylpropyl)aminomethyl, 2-(N,N-dimethylamino)ethyl, 2-(N,N-diethylamino)ethyl, 2-(N,N-dipropylamino)ethyl, 2-[N,N-di(1-methylethyl)amino]ethyl, 2-[N,N-dibutylamino]ethyl, 2-[N,N-di(1-methylpropyl)amino]ethyl, 2-[N,N-di(2-methylpropyl)amino]ethyl, 2-[N,N-di(1,1-dimethylethyl)amino]ethyl, 2-[N-ethyl-N-methylamino]ethyl,

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- C₁-C₄-alkoxy-C₁-C₄-alkyl: C₁-C₄-alkyl which is substituted by C₁-C₄-alkoxy as mentioned above, for example methoxymethyl, ethoxymethyl, propoxymethyl, (1-methylethoxy)methyl, butoxymethyl, (1-methylpropoxy)methyl, (2-methylpropoxy)methyl, (1,1-dimethylethoxy)methyl, 2-(methoxy)ethyl, 2-(ethoxy)ethyl, 2-(propoxy)ethyl, 2-(1-methylethoxy)ethyl, 2-(butoxy)ethyl, 2-(1-methylpropoxy)ethyl, 2-(2-methylpropoxy)ethyl, 2-(1,1-dimethylethoxy)ethyl, 2-(methoxy)-propyl, 2-(ethoxy)propyl, 2-(propoxy)propyl, 2-(1-methylethoxy)propyl, 2-(butoxy)propyl, 2-(1-methylpropoxy)propyl, 2-(2-methylpropoxy)propyl, 2-(1,1-dimethylethoxy)propyl, 3-(methoxy)propyl, 3-(ethoxy)-propyl, 3-(propoxy)propyl, 3-(1-methylethoxy)propyl, 3-(butoxy)propyl, 3-(1-methylpropoxy)propyl, 3-(2-methylpropoxy)propyl, 3-(1,1-dimethylethoxy)propyl, 2-(methoxy)butyl,

- 2-(ethoxy)butyl, 2-(propoxy)butyl, 2-(1-methylethoxy)butyl,
 2-(butoxy)butyl, 2-(1-methylpropoxy)butyl,
 2-(2-methylpropoxy)butyl, 2-(1,1-dimethylethoxy)butyl,
 3-(methoxy)butyl, 3-(ethoxy)butyl, 3-(propoxy)butyl,
 5 3-(1-methylethoxy)butyl, 3-(butoxy)butyl,
 3-(1-methylpropoxy)butyl, 3-(2-methylpropoxy)butyl,
 3-(1,1-dimethylethoxy)butyl, 4-(methoxy)butyl,
 4-(ethoxy)butyl, 4-(propoxy)butyl, 4-(1-methylethoxy)butyl,
 4-(butoxy)butyl, 4-(1-methylpropoxy)butyl,
 10 4-(2-methylpropoxy)butyl and 4-(1,1-dimethylethoxy)butyl;
- C₁-C₄-alkylthio-C₁-C₄-alkyl: C₁-C₄-alkyl which is substituted
 by C₁-C₄-alkylthio as mentioned above, for example
 methylthiomethyl, ethylthiomethyl, propylthiomethyl,
 15 (1-methylethylthio)methyl, butylthiomethyl,
 (1-methylpropylthio)methyl, (2-methylpropylthio)methyl,
 (1,1-dimethylethylthio)methyl, 2-methylthioethyl,
 2-ethylthioethyl, 2-(propylthio)ethyl,
 2-(1-methylethylthio)ethyl, 2-(butylthio)ethyl,
 20 2-(1-methylpropylthio)ethyl, 2-(2-methylpropylthio)ethyl,
 2-(1,1-dimethylethylthio)ethyl, 2-(methylthio)propyl,
 3-(methylthio)propyl, 2-(ethylthio)propyl,
 3-(ethylthio)propyl, 3-(propylthio)propyl,
 3-(butylthio)propyl, 4-(methylthio)butyl, 4-(ethylthio)butyl,
 25 4-(propylthio)butyl and 4-(butylthio)butyl;
- C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl: C₁-C₄-alkyl which is
 substituted by C₁-C₄-alkoxycarbonyl as mentioned above, for
 example methoxycarbonylmethyl, ethoxycarbonylmethyl,
 30 propoxycarbonylmethyl, (1-methylethoxycarbonyl)methyl,
 butoxycarbonylmethyl, (1-methylpropoxycarbonyl)methyl,
 (2-methylpropoxycarbonyl)methyl,
 (1,1-dimethylethoxycarbonyl)methyl, 2-(methoxycarbonyl)ethyl,
 2-(ethoxycarbonyl)ethyl, 2-(propoxycarbonyl)ethyl,
 35 2-(1-methylethoxycarbonyl)ethyl, 2-(butoxycarbonyl)ethyl,
 2-(1-methylpropoxycarbonyl)ethyl,
 2-(2-methylpropoxycarbonyl)ethyl,
 2-(1,1-dimethylethoxycarbonyl)ethyl,
 2-(methoxycarbonyl)propyl, 2-(ethoxycarbonyl)propyl,
 40 2-(propoxycarbonyl)propyl, 2-(1-methylethoxycarbonyl)propyl,
 2-(butoxycarbonyl)propyl, 2-(1-methylpropoxycarbonyl)propyl,
 2-(2-methylpropoxycarbonyl)propyl,
 2-(1,1-dimethylethoxycarbonyl)propyl,
 3-(methoxycarbonyl)propyl, 3-(ethoxycarbonyl)propyl,
 45 3-(propoxycarbonyl)propyl, 3-(1-methylethoxycarbonyl)propyl,
 3-(butoxycarbonyl)propyl, 3-(1-methylpropoxycarbonyl)propyl,
 3-(2-methylpropoxycarbonyl)propyl,

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- 3-(1,1-dimethylethoxycarbonyl)propyl,
 2-(methoxycarbonyl)butyl, 2-(ethoxycarbonyl)butyl,
 2-(propoxycarbonyl)butyl, 2-(1-methylethoxycarbonyl)butyl,
 2-(butoxycarbonyl)butyl, 2-(1-methylpropoxycarbonyl)butyl,
 5 2-(2-methylpropoxycarbonyl)butyl,
 2-(1,1-dimethylethoxycarbonyl)butyl,
 3-(methoxycarbonyl)butyl, 3-(ethoxycarbonyl)butyl,
 3-(propoxycarbonyl)butyl, 3-(1-methylethoxycarbonyl)butyl,
 3-(butoxycarbonyl)butyl, 3-(1-methylpropoxycarbonyl)butyl,
 10 3-(2-methylpropoxycarbonyl)butyl,
 3-(1,1-dimethylethoxycarbonyl)butyl, 4-(methoxycarbonyl)-
 butyl, 4-(ethoxycarbonyl)butyl, 4-(propoxycarbonyl)butyl,
 4-(1-methylethoxycarbonyl)butyl, 4-(butoxycarbonyl)butyl,
 4-(1-methylpropoxy)butoxy, 4-(2-methylpropoxy)butoxy und
 15 4-(1,1-dimethylethoxycarbonyl)butyl;
- C₁-C₄-alkoxy-C₂-C₄-alkoxy: C₂-C₄-alkoxy which is substituted
 by C₁-C₄-alkoxy as mentioned above, for example
 20 2-(methoxy)ethoxy, 2-(ethoxy)ethoxy, 2-(propoxy)ethoxy,
 2-(1-methylethoxy)ethoxy, 2-(butoxy)ethoxy,
 2-(1-methylpropoxy)ethoxy, 2-(2-methylpropoxy)ethoxy,
 2-(1,1-dimethylethoxy)ethoxy, 2-(methoxy)propoxy,
 2-(ethoxy)propoxy, 2-(propoxy)propoxy,
 25 2-(1-methylethoxy)propoxy, 2-(butoxy)propoxy,
 2-(1-methylpropoxy)propoxy, 2-(2-methylpropoxy)propoxy,
 2-(1,1-dimethylethoxy)propoxy, 3-(methoxy)propoxy,
 3-(ethoxy)propoxy, 3-(propoxy)propoxy,
 3-(1-methylethoxy)propoxy, 3-(butoxy)propoxy,
 3-(1-methylpropoxy)propoxy, 3-(2-methylpropoxy)propoxy,
 30 3-(1,1-dimethylethoxy)propoxy, 2-(methoxy)butoxy,
 2-(ethoxy)butoxy, 2-(propoxy)butoxy,
 2-(1-methylethoxy)butoxy, 2-(butoxy)butoxy,
 2-(1-methylpropoxy)butoxy, 2-(2-methylpropoxy)butoxy,
 2-(1,1-dimethylethoxy)butoxy, 3-(methoxy)butoxy, 3-(ethoxy)-
 35 butoxy, 3-(propoxy)butoxy, 3-(1-methylethoxy)butoxy,
 3-(butoxy)butoxy, 3-(1-methylpropoxy)butoxy,
 3-(2-methylpropoxy)butoxy, 3-(1,1-dimethylethoxy)butoxy,
 4-(methoxy)butoxy, 4-(ethoxy)butoxy, 4-(propoxy)butoxy,
 4-(1-methylethoxy)butoxy, 4-(butoxy)butoxy,
 40 4-(1-methylpropoxy)butoxy, 4-(2-methylpropoxy)butoxy and
 4-(1,1-dimethylethoxy)butoxy;
- C₂-C₆-alkanediyl: for example ethane-1,2-diyl,
 45 propane-1,3-diyl, butane-1,4-diyl, pentane-1,5-diyl and
 hexane-1,6-diyl;

- C₃-C₈-cycloalkyl: for example cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl or cyclooctyl;

5 All phenyl rings are preferably unsubstituted or have attached to them one to three halogen atoms and/or a nitro group, a cyano radical and/or one or two methyl, trifluoromethyl, methoxy or trifluoromethoxy substituents.

10 Preference is given to the 3-heterocyclyl-substituted benzoyl derivatives of the formula I where the variables have the following meanings:

15 R¹, R² are hydrogen, nitro, halogen, cyano, C₁-C₆-alkyl, C₁-C₆-haloalkyl, C₁-C₆-alkoxy, C₁-C₆-haloalkoxy, C₁-C₆-alkylthio, C₁-C₆-haloalkylthio, C₁-C₆-alkylsulfinyl, C₁-C₆-haloalkylsulfinyl, C₁-C₆-alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;

20 R³ is hydrogen, halogen or C₁-C₆-alkyl;

25 R⁴, R⁵ are hydrogen, halogen, cyano, nitro, C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, di(C₁-C₄-alkoxy)-C₁-C₄-alkyl, di(C₁-C₄-alkyl)-amino-C₁-C₄-alkyl, [2,2-di(C₁-C₄-alkyl)-1-hydrazino]-C₁-C₄-alkyl, C₁-C₆-alkyliminoxy-C₁-C₄-alkyl, C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl, C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy, 30 C₁-C₄-haloalkoxy, C₁-C₄-alkylthio, C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be fully or partially halogenated and/or to have attached to them one to three of the following groups: 35 nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

or

40 R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

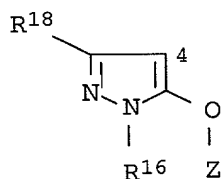
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or

19

- R⁴ and R⁵ together with the corresponding carbon form a carbonyl or thiocarbonyl group;
- 5 R⁶ is C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy, C₃-C₆-alkenyloxy, C₃-C₆-alkynyloxy or NR⁷R⁸;
- R⁷ is hydrogen or C₁-C₄-alkyl;
- 10 R⁸ is C₁-C₄-alkyl;
- X is O, S, NR⁹, CO or CR¹⁰R¹¹;
- 15 Y is O, S, NR¹², CO or CR¹³R¹⁴;
- R⁹, R¹² are hydrogen or C₁-C₄-alkyl;
- 20 R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or CONR⁷R⁸;
- or
- 25 R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or interrupted by oxygen or by a nitrogen which is unsubstituted or
- 30 substituted by C₁-C₄-alkyl;
- R¹⁵ is a pyrazole of the formula II which is linked in the 4-position

35



II

40

where

45

R¹⁶ is C₁-C₆-alkyl;

Z is H or SO₂R¹⁷;

5 R¹⁷ is C₁-C₄-alkyl, C₁-C₄-haloalkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups:
nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

10 R¹⁸ is hydrogen or C₁-C₆-alkyl;

where X and Y are not simultaneously oxygen or sulfur;

15 with the exception of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-ethyl-5-hydroxy-1H-pyrazole,
4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
20 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and
4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;

25 or the agriculturally useful salts thereof.

With a view to the use of the compounds of the formula I
30 according to the invention as herbicides, the variables preferably have the following meanings, in each case alone or in combination:

R¹, R² are nitro, halogen, cyano, C₁-C₆-alkyl,
35 C₁-C₆-haloalkyl, C₁-C₆-alkoxy, C₁-C₆-haloalkoxy, C₁-C₆-alkylthio, C₁-C₆-haloalkylthio, C₁-C₆-alkylsulfinyl, C₁-C₆-haloalkylsulfinyl, C₁-C₆-alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;
especially preferably nitro, halogen such as, for example, chlorine and bromine, C₁-C₆-alkyl such as, for
40 example, methyl and ethyl, C₁-C₆-alkoxy such as, for example, methoxy and ethoxy, C₁-C₆-haloalkyl such as, for example, difluoromethyl and trifluoromethyl, C₁-C₆-alkylthio such as, for example, methylthio and ethylthio, C₁-C₆-alkylsulfinyl such as, for example,
45 methylsulfinyl and ethylsulfinyl, C₁-C₆-alkylsulfonyl such as, for example, methylsulfonyl, ethylsulfonyl and

R⁴, R⁵ are hydrogen, halogen, cyano, nitro, C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, di(C₁-C₄-alkoxy)-C₁-C₄-alkyl, di(C₁-C₄-alkyl)amino-C₁-C₄-alkyl, [2,2-di(C₁-C₄-alkyl)hydrazino-1]-C₁-C₄-alkyl, C₁-C₆-alkyliminooxy-C₁-C₄-alkyl, C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl, C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy, C₁-C₄-alkylthio, C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be partially or fully halogenated and/or to have attached to them one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

R⁴ and R⁵ especially preferably form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

45 R⁷ is hydrogen or C₁-C₄-alkyl;

22

R⁸ is C₁-C₄-alkyl;

X is O, S, NR⁹, CO or CR¹⁰R¹¹;

5 Y is O, S, NR¹² or CR¹³R¹⁴;

R⁹, R¹² are hydrogen or C₁-C₄-alkyl;

10 R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or CONR⁷R⁸;

or

15

R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

20

R¹⁶ is C₁-C₆-alkyl; especially preferably methyl, ethyl, propyl, 2-methylpropyl or butyl;

25

Z is H or SO₂R¹⁷;

30 R¹⁷ is C₁-C₄-alkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

35

R¹⁸ is hydrogen or C₁-C₆-alkyl; especially preferably hydrogen or methyl.

The following embodiments of the 3-heterocyclyl-substituted benzoyl derivatives of the formula I must be emphasized:

40

1. In a preferred embodiment of the 3-heterocyclyl-substituted benzoyl derivatives of the formula I, Z is SO₂R¹⁷.

45

- R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by

24

oxygen or by a nitrogen which is unsubstituted
or substituted by C₁-C₄-alkyl;

or

5

R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain
which can be mono- to tetrasubstituted by
C₁-C₄-alkyl and/or which can be interrupted by
oxygen or by a nitrogen which is unsubstituted
or substituted by C₁-C₄-alkyl.

10

- Extraordinarily preferred are 3-heterocyclyl-
substituted benzoyl derivatives of the formula I
where

15

R⁴ is C₁-C₄-alkyl, C₁-C₄-haloalkyl,
C₁-C₄-alkoxycarbonyl or CONR⁷R⁸;

20

R⁵ is hydrogen or C₁-C₄-alkyl;

or

25

R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain
which can be mono- to tetrasubstituted by
C₁-C₄-alkyl and/or which can be interrupted by
oxygen or by a nitrogen which is unsubstituted
or substituted by C₁-C₄-alkyl;

30

or

35

R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain
which can be mono- to tetrasubstituted by
C₁-C₄-alkyl and/or which can be interrupted by
oxygen or by a nitrogen which is unsubstituted
or substituted by C₁-C₄-alkyl.

40

Especially extraordinarily preferred are
3-heterocyclyl-substituted benzoyl derivatives of the
formula I where R¹⁸ is hydrogen.

- * Also particularly preferred are
3-heterocyclyl-substituted benzoyl derivatives of the
formula I where R⁴ and R⁵ are hydrogen.

45

25

- Extraordinarily preferred are 3-heterocyclyl-substituted benzoyl derivatives of the formula I where R¹⁸ is hydrogen.

5 Especially extraordinarily preferred are 3-heterocyclyl-substituted benzoyl derivatives of the formula I where

10 R¹ is nitro, C₁-C₆-alkyl such as, for example, methyl and ethyl, C₁-C₆-alkoxy such as, for example, methoxy and ethoxy, C₁-C₆-haloalkyl such as, for example, difluoromethyl and trifluoromethyl, C₁-C₆-alkylsulfonyl such as, for example, methylsulfonyl, 15 ethylsulfonyl and propylsulfonyl, or C₁-C₆-haloalkylsulfonyl such as, for example, trifluoromethylsulfonyl and pentafluoroethylsulfonyl;

20 Also especially extraordinarily preferred are 3-heterocyclyl-substituted benzoyl derivatives of the formula I where

25 R² is nitro, halogen such as, for example, chlorine and bromine, C₁-C₆-alkyl such as, for example, methyl and ethyl, C₁-C₆-haloalkyl such as, for example, difluoromethyl and trifluoromethyl, 30 C₁-C₆-alkylthio such as, for example, methylthio and ethylthio, C₁-C₆-alkylsulfinyl such as, for example, methylsulfinyl and ethylsulfinyl, C₁-C₆-alkylsulfonyl such as, for example, 35 methylsulfonyl, ethylsulfonyl and propylsulfonyl, or C₁-C₆-haloalkylsulfonyl such as, for example, trifluoromethylsulfonyl and pentafluoroethylsulfonyl.

40 Also especially extraordinarily preferred is 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-methyl-5-hydroxy-1H-pyrazole.

45

Also especially extraordinarily preferred are the agriculturally useful salts of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-methyl-5-hydroxy-1H-pyrazole, in particular the alkali metal salts, such as, for example, lithium, sodium and potassium, and the ammonium salts, it being possible in this case, if desired, for one to four hydrogen atoms to be replaced by C₁-C₄-alkyl, hydroxy-C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, hydroxy-C₁-C₄-alkoxy-C₁-C₄-alkyl, phenyl or benzyl, preferably ammonium, dimethylammonium, diisopropylammonium, tetramethylammonium, tetrabutylammonium, 2-(2-hydroxyeth-1-oxy)eth-1-ylammonium, di(2-hydroxyeth-1-yl)ammonium, trimethylbenzylammonium.

- Also extraordinarily preferred are 3-heterocycl-yl-substituted benzoyl derivatives of the formula I where R¹⁸ is methyl.

Especially extraordinarily preferred are 3-heterocycl-yl-substituted benzoyl derivatives of the formula I where

R¹ is nitro, C₁-C₆-alkyl such as, for example, methyl and ethyl, C₁-C₆-alkoxy such as, for example, methoxy and ethoxy, C₁-C₆-haloalkyl such as, for example, difluoromethyl and trifluoromethyl, C₁-C₆-alkylsulfonyl such as, for example, methylsulfonyl, ethylsulfonyl and propylsulfonyl, or C₁-C₆-haloalkylsulfonyl, for example trifluoromethylsulfonyl and pentafluoroethylsulfonyl.

Also especially extraordinarily preferred are 3-heterocycl-yl-substituted benzoyl derivatives of the formula I where

R² is nitro, halogen such as, for example, chlorine and bromine, C₁-C₆-alkyl such as, for example, methyl and ethyl, C₁-C₆-haloalkyl such as, for example, difluoromethyl and trifluoromethyl, C₁-C₆-alkylthio such as, for example,

27

methylthio and ethylthio,
 C₁-C₆-alkylsulfinyl such as, for example,
 methylsulfinyl and ethylsulfinyl,
 C₁-C₆-alkylsulfonyl such as, for example,
 methylsulfonyl, ethylsulfonyl and
 propylsulfonyl, or C₁-C₆-haloalkylsulfonyl
 such as, for example,
 trifluoromethylsulfonyl and
 pentafluoroethylsulfonyl.

- Also especially preferred are 3-heterocyclyl-substituted
 benzoyl derivatives of the formula I where

X is S, NR⁹, CO or CR¹⁰R¹¹;

or

Y is O, S, NR¹² or CO.

* Particularly preferred are 3-heterocyclyl-substituted
 benzoyl derivatives of the formula I where R¹⁸ is
 hydrogen.

* Also particularly preferred are 3-heterocyclyl-
 substituted benzoyl derivatives of the formula I
 where R¹⁸ is C₁-C₆-alkyl.

• Extraordinarily preferred are 3-heterocyclyl-
 substituted benzoyl derivatives of the formula I
 where

R⁴ is halogen, cyano, nitro, C₁-C₄-alkyl,
 C₁-C₄-alkoxy-C₁-C₄-alkyl,
 C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl,
 C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl,
 C₁-C₆-alkoxy, C₁-C₄-alkoxy-C₁-C₄-alkoxy,
 C₁-C₄-haloalkoxy, C₁-C₄-alkylthio,
 C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino,
 COR⁶, phenyl or benzyl, it being possible
 for the two last-mentioned substituents to
 be partially or fully halogenated and/or to
 have attached to them one to three of the
 following groups:

28

nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

5 R⁵ is hydrogen or C₁-C₄-alkyl;

or

10 R⁴ and R⁵ together form a C₂-C₆-alkanediyl
chain which can be mono- to tetrasubstituted
by C₁-C₄-alkyl and/or which can be
interrupted by oxygen or by a nitrogen which
is unsubstituted or substituted by
C₁-C₄-alkyl;

15

or

20 R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and
R¹³ together form a C₂-C₆-alkanediyl chain
which can be mono- to tetrasubstituted by
C₁-C₄-alkyl and/or which can be interrupted
by oxygen or by a nitrogen which is
unsubstituted or substituted by C₁-C₄-alkyl.

25

* Also particularly preferred are 3-heterocyclyl-
substituted benzoyl derivatives of the formula I
where

30

X is S, NR⁹ or CO

or

35

Y is O, NR¹² or CO.

40

• Extraordinarily preferred are 3-heterocyclyl-
substituted benzoyl derivatives of the formula I
where

45

R⁴ is halogen, cyano, nitro, C₁-C₄-alkyl,
C₁-C₄-alkoxy-C₁-C₄-alkyl,
C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl,
C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl,
C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl,
C₁-C₆-alkoxy, C₁-C₄-alkoxy-C₁-C₄-alkoxy,
C₁-C₄-haloalkoxy, C₁-C₄-alkylthio,

29

C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be partially or fully halogenated and/or to have attached to them one to three of the following groups:

nitro, cyano, C₁-C₄-Alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

10 R⁵ is hydrogen or C₁-C₄-alkyl;

or

15 R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by
20 C₁-C₄-alkyl;

or

25 R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is
30 unsubstituted or substituted by C₁-C₄-alkyl.

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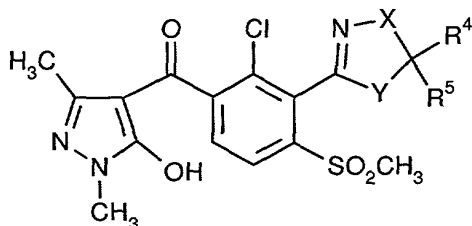
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Particularly extraordinarily preferred are the compounds Ia1 (\cong I where $R^1 = Cl$, $R^2 = SO_2CH_3$, $R^3 = H$, R^{16} , $R^{18} = CH_3$, $Z=H$), in particular the compounds of Table 1.

5

10



Ia1

15 Table 1

No.	X	R ⁴	R ⁵	Y
Ia1.1	CH ₂	H	CH ₃	O
Ia1.2	CH ₂	H	H	O
Ia1.3	C(CH ₃) ₂	H	H	O
Ia1.4	CH ₂	H	C ₂ H ₅	O
Ia1.5	CH ₂	CH ₃	CH ₃	O
Ia1.6	CH(CH ₃)	H	CH ₃	O
Ia1.7	CH(C ₂ H ₅)	H	CH ₃	O
Ia1.8	CH[CH(CH ₃) ₂]	H	H	O
Ia1.9	CH ₂	H	CH(CH ₃) ₂	O
Ia1.10	CH(C ₂ H ₅)	H	C ₂ H ₅	O
Ia1.11	-CH-(CH ₂) ₄ -		H	O
Ia1.12	C=O	CH ₃	CH ₃	O
Ia1.13	C=O	H	C ₂ H ₅	O
Ia1.14	C=O	C ₂ H ₅	C ₂ H ₅	O
Ia1.15	C=O	H	H	O
Ia1.16	C=O	H	CH ₃	O
Ia1.17	CH ₂	H	CH ₃	S
Ia1.18	C(CH ₃) ₂	H	H	S
Ia1.19	CH ₂	H	C ₂ H ₅	S
Ia1.20	CH ₂	CH ₃	CH ₃	S
Ia1.21	CH(CH ₃)	H	CH ₃	S
Ia1.22	CH(C ₂ H ₅)	H	CH ₃	S
Ia1.23	CH(C ₂ H ₅)	H	C ₂ H ₅	S
Ia1.24	-CH-(CH ₂) ₄ -		H	S
Ia1.25	CH[CH(CH ₃) ₂]	H	H	S
Ia1.26	CH ₂	H	CH(CH ₃) ₂	S
Ia1.27	CH ₂	H	CH ₃	NH
Ia1.28	CH ₂	H	H	NH
Ia1.29	C(CH ₃) ₂	H	H	NH
Ia1.30	CH ₂	H	C ₂ H ₅	NH
Ia1.31	CH ₂	CH ₃	CH ₃	NH

45

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No.	X	R ⁴	R ⁵	Y
5	la1.32	CH(CH ₃)	CH ₃	NH
	la1.33	CH(C ₂ H ₅)	CH ₃	NH
	la1.34	CH(C ₂ H ₅)	C ₂ H ₅	NH
	la1.35	-CH-(CH ₂) ₄ -	H	NH
	la1.36	CH[CH(CH ₃) ₂]	H	NH
10	la1.37	CH ₂	CH(CH ₃) ₂	NH
	la1.38	CH ₂	CH ₃	NCH ₃
	la1.39	CH ₂	H	NCH ₃
	la1.40	C(CH ₃) ₂	H	NCH ₃
	la1.41	CH ₂	C ₂ H ₅	NCH ₃
15	la1.42	CH ₂	CH ₃	NCH ₃
	la1.43	CH(CH ₃)	CH ₃	NCH ₃
	la1.44	CH(C ₂ H ₅)	CH ₃	NCH ₃
	la1.45	CH[CH(CH ₃) ₂]	H	NCH ₃
	la1.46	CH ₂	CH(CH ₃) ₂	NCH ₃
20	la1.47	CH(C ₂ H ₅)	C ₂ H ₅	NCH ₃
	la1.48	-CH-(CH ₂) ₄ -	H	NCH ₃
	la1.49	CH ₂	CH ₃	NC ₂ H ₅
	la1.50	CH ₂	H	NC ₂ H ₅
	la1.51	C(CH ₃) ₂	H	NC ₂ H ₅
25	la1.52	CH ₂	C ₂ H ₅	NC ₂ H ₅
	la1.53	CH ₂	CH ₃	NC ₂ H ₅
	la1.54	CH(CH ₃)	CH ₃	NC ₂ H ₅
	la1.55	CH(C ₂ H ₅)	CH ₃	NC ₂ H ₅
	la1.56	CH[CH(CH ₃) ₂]	H	NC ₂ H ₅
30	la1.57	CH ₂	CH(CH ₃) ₂	NC ₂ H ₅
	la1.58	CH(C ₂ H ₅)	C ₂ H ₅	NC ₂ H ₅
	la1.59	-CH-(CH ₂) ₄ -	H	NC ₂ H ₅
	la1.60	CH ₂	=O	S
	la1.61	CH(CH ₃)	=O	S
35	la1.62	CH(C ₂ H ₅)	=O	S
	la1.63	CH[CH(CH ₃) ₂]	=O	S
	la1.64	C(CH ₃) ₂	=O	S
	la1.65	CCH ₃ (C ₂ H ₅)	=O	S
	la1.66	CCH ₃ [CH(CH ₃) ₂]	=O	S
40	la1.67	CH ₂	=O	NH
	la1.68	CH(CH ₃)	=O	NH
	la1.69	CH(C ₂ H ₅)	=O	NH
	la1.70	CH[CH(CH ₃) ₂]	=O	NH
	la1.71	C(CH ₃) ₂	=O	NH
45	la1.72	CCH ₃ (C ₂ H ₅)	=O	NH
	la1.73	CCH ₃ [CH(CH ₃) ₂]	=O	NH
	la1.74	CH ₂	=O	NCH ₃
	la1.75	CH(CH ₃)	=O	NCH ₃
	la1.76	CH(C ₂ H ₅)	=O	NCH ₃
	la1.77	CH[CH(CH ₃) ₂]	=O	NCH ₃

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No.	X	R ⁴	R ⁵	Y	
	Ia1.78	C(CH ₃) ₂	=O	NCH ₃	
	Ia1.79	CCH ₃ (C ₂ H ₅)	=O	NCH ₃	
5	Ia1.80	CCH ₃ [CH(CH ₃) ₂]	=O	NCH ₃	
	Ia1.81	O	COOCH ₃	H	CH ₂
	Ia1.82	O	COOC ₂ H ₅	H	CH ₂
	Ia1.83	O	CONHCH ₃	H	CH ₂
	Ia1.84	O	CON(CH ₃) ₂	H	CH ₂
10	Ia1.85	O	CONHC ₂ H ₅	H	CH ₂
	Ia1.86	O	CON(C ₂ H ₅) ₂	H	CH ₂
	Ia1.87	O	CH ₃	H	CH ₂
	Ia1.88	O	C ₂ H ₅	H	CH ₂
	Ia1.89	O	CH(CH ₃) ₂	H	CH ₂
15	Ia1.90	O	COC ₂ H ₅	H	CH ₂
	Ia1.91	O	CH ₂ CN	H	CH ₂
	Ia1.92	O	CH ₂ N(CH ₃) ₂	H	CH ₂
	Ia1.93	O	CH ₂ ON=C(CH ₃) ₂	H	CH ₂
	Ia1.94	O	CH(OC ₂ H ₅) ₂	H	CH ₂
	Ia1.95	O	CH(OCH ₃) ₂	H	CH ₂
20	Ia1.96	O	CH ₃	CH ₃	CH ₂
	Ia1.97	O	CH ₃	C ₂ H ₅	CH ₂
	Ia1.98	O	C ₂ H ₅	C ₂ H ₅	CH ₂
	Ia1.99	O	-(CH ₂) ₄ -		CH ₂
	Ia1.100	O	-(CH ₂) ₂ -O-(CH ₂) ₂ -		CH ₂
25	Ia1.101	O	H	-(CH ₂) ₃ -CH-	
	Ia1.102	O	H	-(CH ₂) ₄ -CH-	
	Ia1.103	O	CH ₃	H	CHCH ₃
	Ia1.104	S	=O		O
	Ia1.105	CH ₂	=S		S
30	Ia1.106	CH(CH ₃)	=S		S
	Ia1.107	CH(C ₂ H ₅)	=S		S
	Ia1.108	C(CH ₃) ₂	=S		S
	Ia1.109	O	=O		NH
	Ia1.110	O	=O		NCH ₃
35	Ia1.111	O	CH ₃	H	NH
	Ia1.112	O	C ₂ H ₅	H	NH
	Ia1.113	O	CH ₃	CH ₃	NH
	Ia1.114	O	C ₂ H ₅	C ₂ H ₅	NH
	Ia1.115	O	CH ₃	H	NCH ₃
40	Ia1.116	O	C ₂ H ₅	H	NCH ₃
	Ia1.117	O	CH ₃	CH ₃	NCH ₃
	Ia1.118	O	C ₂ H ₅	C ₂ H ₅	NCH ₃
	Ia1.119	NH	=O		NH
	Ia1.120	NH	=O		NCH ₃
45	Ia1.121	NCH ₃	=O		NH
	Ia1.122	NCH ₃	=O		NCH ₃

REF ID: A66660

In addition, the following benzoyl derivatives of the formula I are particularly extraordinarily preferred:

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No.	X	R ⁴	R ⁵	Y
		$-\text{CH}-(\text{CH}_2)_4-$	H	O
			CH ₃	O
5	Ib1.12	C=O	CH ₃	O
	Ib1.13	C=O	H	O
	Ib1.14	C=O	C ₂ H ₅	O
	Ib1.15	C=O	C ₂ H ₅	O
	Ib1.16	C=O	H	O
	Ib1.17	C=O	CH ₃	O
	Ib1.18	CH ₂	CH ₃	S
10	Ib1.19	CH ₂	H	S
	Ib1.20	C(CH ₃) ₂	H	S
	Ib1.21	CH ₂	C ₂ H ₅	S
	Ib1.22	CH ₂	CH ₃	S
	Ib1.23	CH(CH ₃)	CH ₃	S
15	Ib1.24	CH(C ₂ H ₅)	CH ₃	S
	Ib1.25	CH(C ₂ H ₅)	C ₂ H ₅	S
	Ib1.26	$-\text{CH}-(\text{CH}_2)_4-$	H	S
	Ib1.27	CH[CH(CH ₃) ₂]	H	S
	Ib1.28	CH ₂	CH(CH ₃) ₂	S
20	Ib1.29	CH ₂	CH ₃	NH
	Ib1.30	CH ₂	H	NH
	Ib1.31	CH ₂	H	NH
	Ib1.32	C(CH ₃) ₂	H	NH
	Ib1.33	CH ₂	C ₂ H ₅	NH
	Ib1.34	CH ₂	CH ₃	NH
25	Ib1.35	CH(CH ₃)	CH ₃	NH
	Ib1.36	CH(C ₂ H ₅)	CH ₃	NH
	Ib1.37	CH(C ₂ H ₅)	C ₂ H ₅	NH
	Ib1.38	$-\text{CH}-(\text{CH}_2)_4-$	H	NH
	Ib1.39	CH[CH(CH ₃) ₂]	H	NH
	Ib1.40	CH ₂	CH(CH ₃) ₂	NH
30	Ib1.41	CH ₂	CH ₃	NCH ₃
	Ib1.42	CH ₂	H	NCH ₃
	Ib1.43	CH ₂	H	NCH ₃
	Ib1.44	C(CH ₃) ₂	H	NCH ₃
	Ib1.45	CH ₂	C ₂ H ₅	NCH ₃
	Ib1.46	CH ₂	CH ₃	NCH ₃
35	Ib1.47	CH(CH ₃)	CH ₃	NCH ₃
	Ib1.48	CH(C ₂ H ₅)	CH ₃	NCH ₃
	Ib1.49	CH[CH(CH ₃) ₂]	H	NCH ₃
	Ib1.50	CH ₂	CH(CH ₃) ₂	NCH ₃
	Ib1.51	CH ₂	C ₂ H ₅	NCH ₃
40	Ib1.52	CH(C ₂ H ₅)	H	NCH ₃
	Ib1.53	$-\text{CH}-(\text{CH}_2)_4-$	CH ₃	NC ₂ H ₅
	Ib1.54	CH ₂	H	NC ₂ H ₅
	Ib1.55	CH ₂	H	NC ₂ H ₅
	Ib1.56	C(CH ₃) ₂	H	NC ₂ H ₅
	Ib1.57	CH ₂	C ₂ H ₅	NC ₂ H ₅
45	Ib1.58	CH ₂	CH ₃	NC ₂ H ₅
	Ib1.59	CH(CH ₃)	CH ₃	NC ₂ H ₅
	Ib1.60	CH(C ₂ H ₅)	CH ₃	NC ₂ H ₅

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No.	X	R ⁴	R ⁵	Y	
5	lb1.57	CH[CH(CH ₃) ₂]	H	NC ₂ H ₅	
	lb1.58	CH ₂	H	NC ₂ H ₅	
	lb1.59	CH(C ₂ H ₅)	H	NC ₂ H ₅	
	lb1.60	-CH-(CH ₂) ₄ -		H	NC ₂ H ₅
	lb1.61	CH ₂	=O		S
10	lb1.62	CH(CH ₃)	=O		S
	lb1.63	CH(C ₂ H ₅)	=O		S
	lb1.64	CH[CH(CH ₃) ₂]	=O		S
	lb1.65	C(CH ₃) ₂	=O		S
	lb1.66	CCH ₃ (C ₂ H ₅)	=O		S
15	lb1.67	CCH ₃ [CH(CH ₃) ₂]	=O		S
	lb1.68	CH ₂	=O		NH
	lb1.69	CH(CH ₃)	=O		NH
	lb1.70	CH(C ₂ H ₅)	=O		NH
	lb1.71	CH[CH(CH ₃) ₂]	=O		NH
20	lb1.72	C(CH ₃) ₂	=O		NH
	lb1.73	CCH ₃ (C ₂ H ₅)	=O		NH
	lb1.74	CCH ₃ [CH(CH ₃) ₂]	=O		NH
	lb1.75	CH ₂	=O		NCH ₃
	lb1.76	CH(CH ₃)	=O		NCH ₃
25	lb1.77	CH(C ₂ H ₅)	=O		NCH ₃
	lb1.78	CH[CH(CH ₃) ₂]	=O		NCH ₃
	lb1.79	C(CH ₃) ₂	=O		NCH ₃
	lb1.80	CCH ₃ (C ₂ H ₅)	=O		NCH ₃
	lb1.81	CCH ₃ [CH(CH ₃) ₂]	=O		NCH ₃
30	lb1.82	O	COOCH ₃	H	CH ₂
	lb1.83	O	COOC ₂ H ₅	H	CH ₂
	lb1.84	O	CONHCH ₃	H	CH ₂
	lb1.85	O	CON(CH ₃) ₂	H	CH ₂
	lb1.86	O	CONHC ₂ H ₅	H	CH ₂
35	lb1.87	O	CON(C ₂ H ₅) ₂	H	CH ₂
	lb1.88	O	CH ₃	H	CH ₂
	lb1.89	O	C ₂ H ₅	H	CH ₂
	lb1.90	O	CH(CH ₃) ₂	H	CH ₂
	lb1.91	O	COC ₂ H ₅	H	CH ₂
40	lb1.92	O	CH ₂ CN	H	CH ₂
	lb1.93	O	CH ₂ N(CH ₃) ₂	H	CH ₂
	lb1.94	O	CH ₂ ON=C(CH ₃) ₂	H	CH ₂
	lb1.95	O	CH(OC ₂ H ₅) ₂	H	CH ₂
	lb1.96	O	CH(OCH ₃) ₂	H	CH ₂
45	lb1.97	O	CH ₃	CH ₃	CH ₂
	lb1.98	O	CH ₃	C ₂ H ₅	CH ₂
	lb1.99	O	C ₂ H ₅	C ₂ H ₅	CH ₂
	lb1.100	O	-(CH ₂) ₄ -		CH ₂
	lb1.101	O	-(CH ₂) ₂ -O-(CH ₂) ₂ -		CH ₂
	lb1.102	O	H	-(CH ₂) ₃ -CH-	

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No.	X	R ⁴	R ⁵	Y
1b1.103	O	H	-(CH ₂) ₄ -CH-	
1b1.104	O	CH ₃	H	CHCH ₃
5 1b1.105	O	H	H	CH ₂
1b1.106	S		=O	O
1b1.107	CH ₂		=S	S
1b1.108	CH(CH ₃)		=S	S
1b1.109	CH(C ₂ H ₅)		=S	S
10 1b1.110	C(CH ₃) ₂		=S	S
1b1.111	O		=O	NH
1b1.112	O		=O	NCH ₃
1b1.113	O	CH ₃	H	NH
1b1.114	O	C ₂ H ₅	H	NH
15 1b1.115	O	CH ₃	CH ₃	NH
1b1.116	O	C ₂ H ₅	C ₂ H ₅	NH
1b1.117	O	CH ₃	H	NCH ₃
1b1.118	O	C ₂ H ₅	H	NCH ₃
1b1.119	O	CH ₃	CH ₃	NCH ₃
20 1b1.120	O	C ₂ H ₅	C ₂ H ₅	NCH ₃
1b1.121	NH		=O	NH
1b1.122	NH		=O	NCH ₃
1b1.123	NCH ₃		=O	NH
1b1.124	NCH ₃		=O	NCH ₃
1b1.125	NC ₂ H ₅		=O	NH
25 1b1.126	NC ₂ H ₅		=O	NC ₂ H ₅

In addition, the following 3-heterocyclyl-substituted benzoyl derivatives of the formula I are particularly extraordinarily preferred:

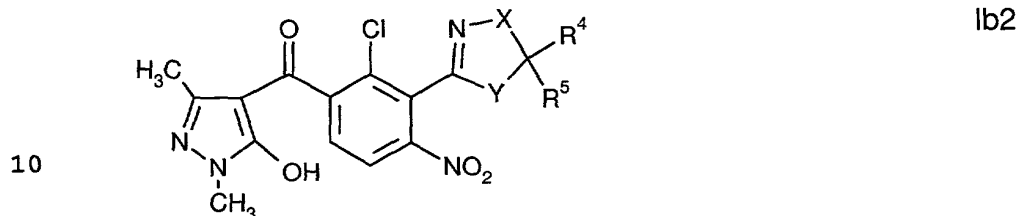
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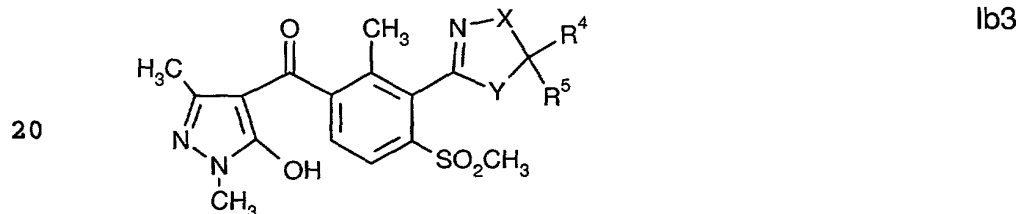
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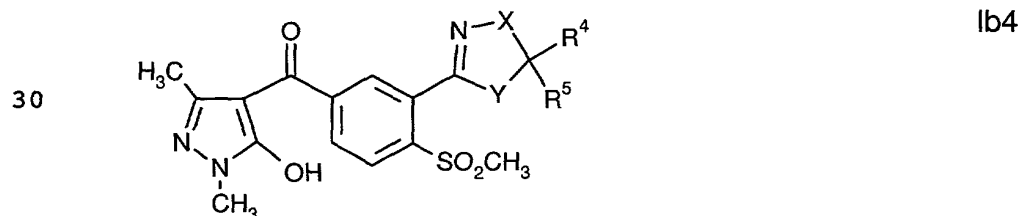
- 5 - The compounds Ib2.1-Ib2.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro.



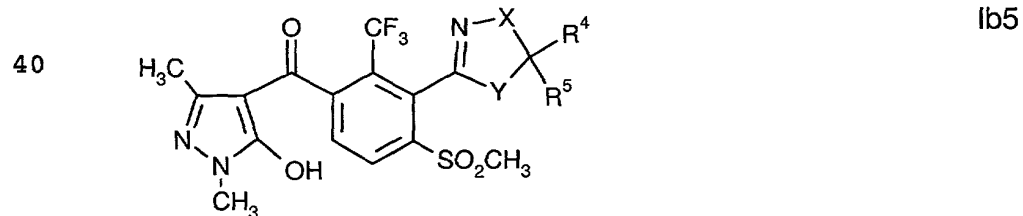
- 15 - The compounds Ib3.1-Ib3.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl and R² is methylsulfonyl.



- 25 - The compounds Ib4.1-Ib4.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact R¹ is hydrogen and R² is methylsulfonyl.



- 35 - The compounds Ib5.1-Ib5.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is trifluoromethyl and R² is methylsulfonyl.



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Chemical structure 39 is a 1,2,4-triazole derivative. The triazole ring is substituted with a methyl group (H₃C) at position 5 and a methylamino group (N-CH₃) at position 3. The triazole is linked via its 4-position to a carbonyl group (C=O), which is further linked to a benzene ring. The benzene ring has a chlorine atom (Cl) at position 1, a methanesulfonyl group (SOCH₃) at position 3, and a 1,2,4-triazol-5-yl group at position 4. The triazole ring in the side chain is substituted with an X group at position 1 and Y and R⁵ groups at position 2, with an R⁴ group attached to the nitrogen at position 1.

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Cc1nc2c(c1)c(O)c(=O)c3cc(Cl)c(C(=N)C(R4)(R5)Y)c(S(=O)(=O)C(F)(F)F)c32 \square^4

- 20

Cc1nc2c(c1)c(O)c(=O)c3cc(OC)c(C(=N[X])(Y)C(R4)R5)c(S(=O)(=O)C)c32

D4

- 30

Cc1nc2c(c1)c(O)c(=O)c3cc(Cl)c(C(=N)C(R4)(R5)Y)c(S(=O)(=O)CC)c3D⁴

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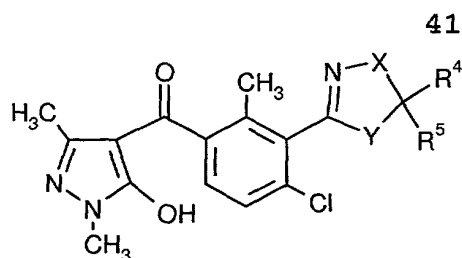


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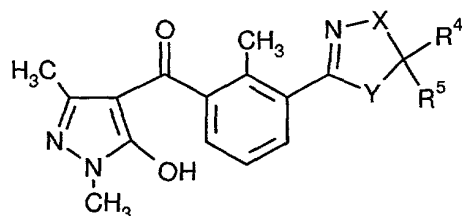


Ib18

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- The compounds Ib19.1-Ib19.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl and R² is hydrogen.

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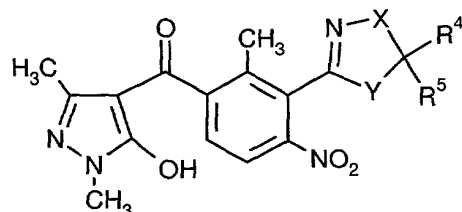


Ib19

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- The compounds Ib20.1-Ib20.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact R¹ is methyl and R² is nitro.

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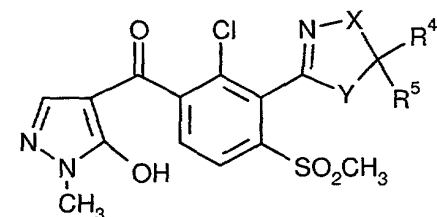


Ib20

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- The compounds Ib21.1-Ib21.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl and R¹⁸ is hydrogen.

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Ib21

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- The compounds Ib22.1-Ib22.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro and R¹⁸ is hydrogen.

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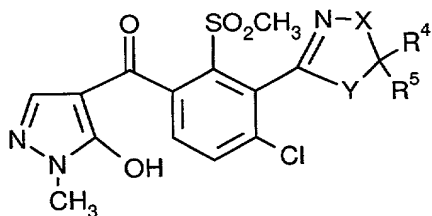
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Ib26

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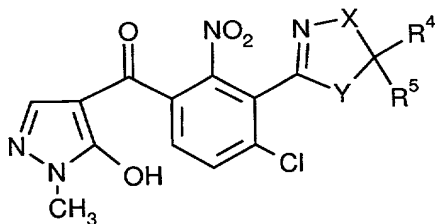


- The compounds Ib27.1-Ib27.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact R^1 is nitro and R^{18} is hydrogen.

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Ib27

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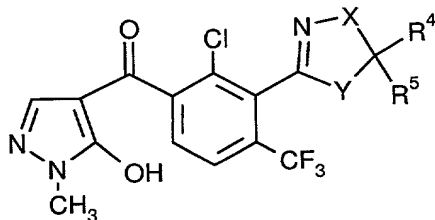


- The compounds Ib28.1-Ib28.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^2 is trifluoromethyl and R^{18} is hydrogen.

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Ib28

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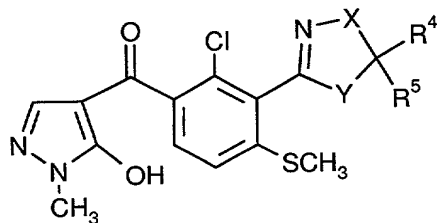


- The compounds Ib29.1-Ib29.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^2 is methylthio and R^{18} is hydrogen.

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Ib29

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- The compounds Ib30.1-Ib30.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^2 is methylsulfinyl and R^{18} is hydrogen.

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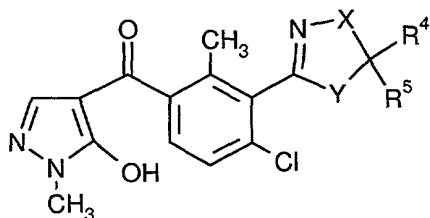


- 45 - The compounds Ib38.1-Ib38.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl and R¹⁸ is hydrogen.

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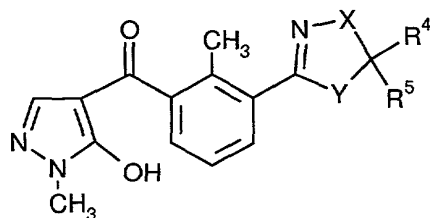
Ib38

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- 10 - The compounds Ib39.1-Ib39.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is hydrogen and R¹⁸ is hydrogen.

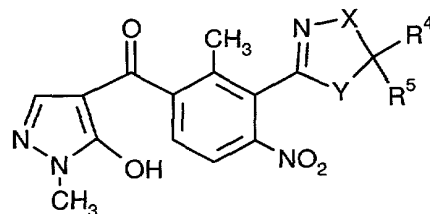
15



Ib39

- 20 - The compounds Ib40.1-Ib40.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is nitro and R¹⁸ is hydrogen.

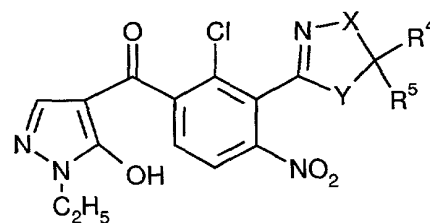
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Ib40

- 30 - The compounds Ib41.1-Ib41.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is ethyl and R¹⁸ is hydrogen.

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Ib41

- 40 - The compounds Ib42.1-Ib42.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

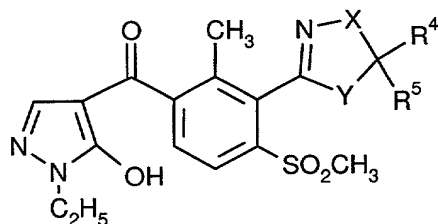
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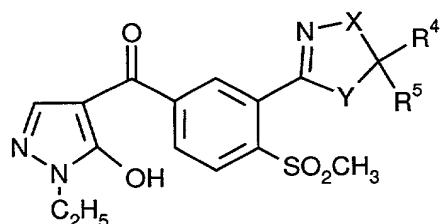
Ib42

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- 10 - The compounds Ib43.1-Ib43.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is hydrogen, R² is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

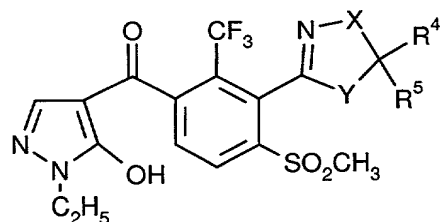
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Ib43

- 20 - The compounds Ib44.1-Ib44.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is trifluoromethyl, R² is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

25

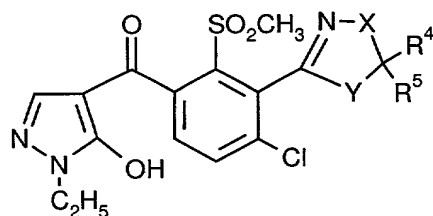


Ib44

30

- 35 - The compounds Ib45.1-Ib45.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

35

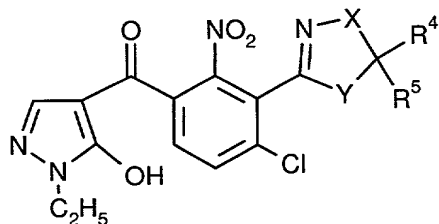


Ib45

40

- 45 - The compounds Ib46.1-Ib46.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl and R¹⁸ is hydrogen.

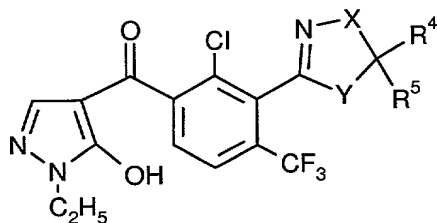
48



- The compounds Ib47.1-Ib47.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

10

b47

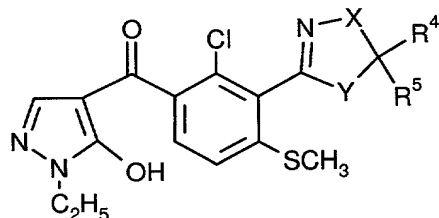


20

- The compounds Ib48.1-Ib48.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylthio, R¹⁶ is ethyl and R¹⁸ is hydrogen.

25

1b48

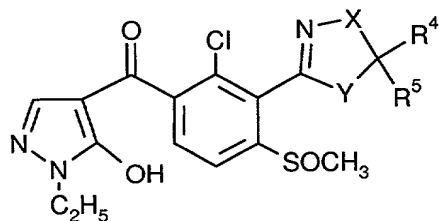


30 -

- The compounds Ib49.1-Ib49.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfinyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

35

b49



40

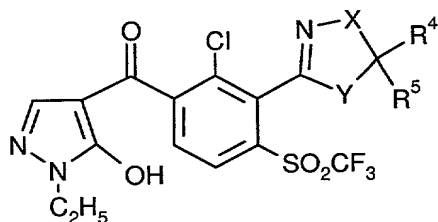
- The compounds Ib50.1-Ib50.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

45

49

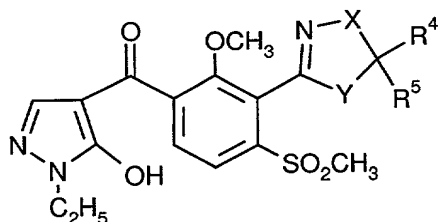
Ib50

5



- 10 - The compounds Ib51.1-Ib51.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

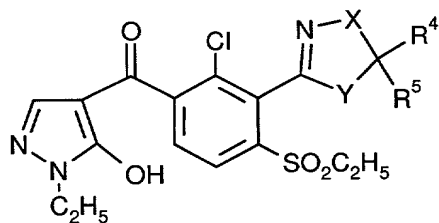
15



Ib51

- 20 - The compounds Ib52.1-Ib52.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

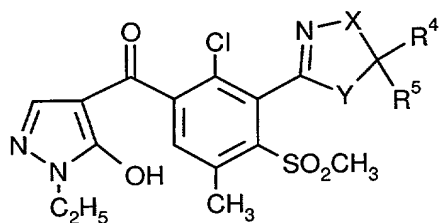
25



Ib52

- 30 - The compounds Ib53.1-Ib53.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is methyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

35



Ib53

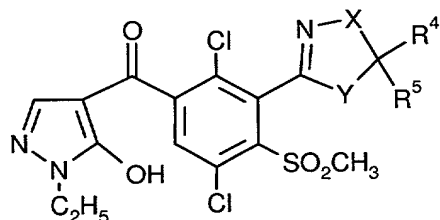
40

- 45 - The compounds Ib54.1-Ib54.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is chlorine, R¹⁶ is ethyl and R¹⁸ is hydrogen.

50

Ib54

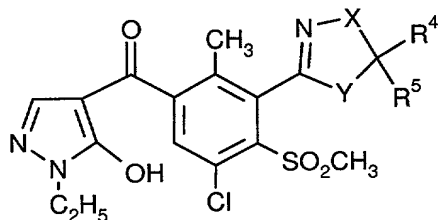
5



- 10 - The compounds Ib55.1-Ib55.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is chlorine, R¹⁶ is ethyl and R¹⁸ is hydrogen.

15

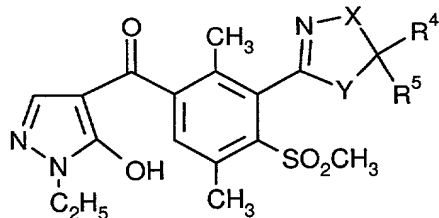
Ib55



- 20 - The compounds Ib56.1-Ib56.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is methyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

25

Ib56

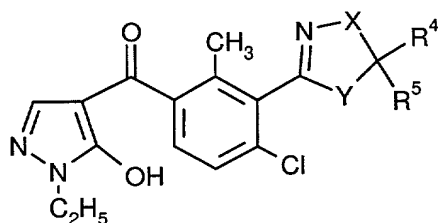


30

- 35 - The compounds Ib57.1-Ib57.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

35

Ib57



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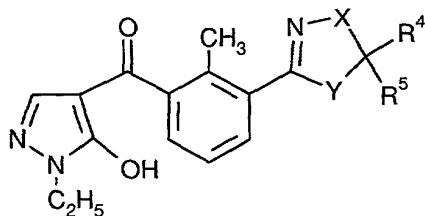
- 45 - The compounds Ib58.1-Ib58.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is hydrogen, R¹⁶ is ethyl and R¹⁸ is hydrogen.

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51

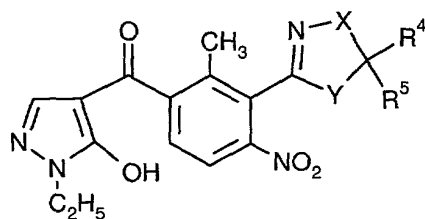
Ib58

5



- 10 - The compounds Ib59.1-Ib59.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is nitro, R¹⁶ is ethyl and R¹⁸ is hydrogen.

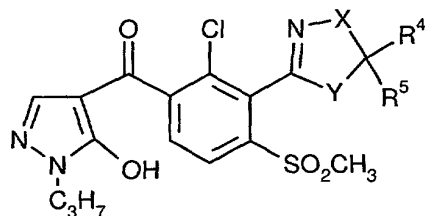
15



Ib59

- 20 - The compounds Ib60.1-Ib60.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

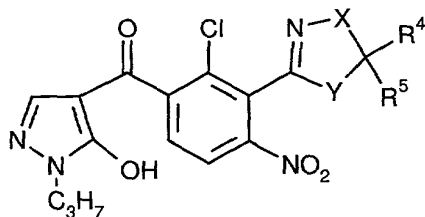
25



Ib60

- 30 - The compounds Ib61.1-Ib61.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

35



Ib61

- 40 - The compounds Ib62.1-Ib62.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

45

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1b62

CC1=CN2C(=C1)C(=O)C(=C2)C(=O)c3ccc(cc3C(=O)N(C)C)S(=O)(=O)C

20 - The compounds Ib64.1-Ib64.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is trifluoromethyl, R² is methylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

CN1C=NC2=C1C(=O)C(=C2)C(=O)c3cc(C(F)(F)F)c(C(=NXC(R4)(R5)Y)c4cc(S(=O)(=O)C)cc4)cc3

30

- The compounds Ib65.1-Ib65.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

CC1=CN2C(=C1)C(=O)C2=C(C(=O)c3cc(Cl)cc(C(=O)N(C)C)c3)S(=O)(=O)C

b6
b7C
b7D

40

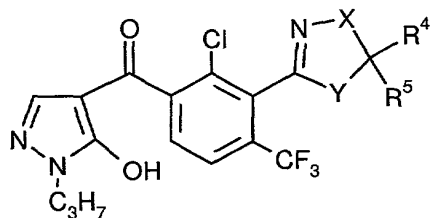
- The compounds Ib66.1-Ib66.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

45

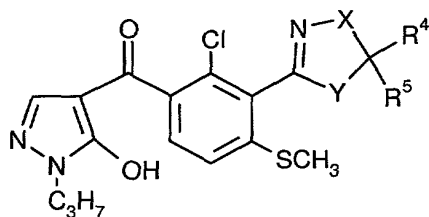
53



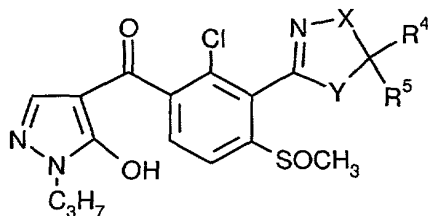
- b6
b7C
b7D



- b6
b7C
b7D



- 1b69



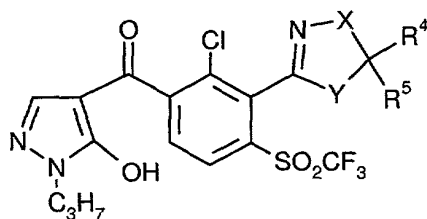
- The compounds Ib70.1-Ib70.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

45

54

Ib70

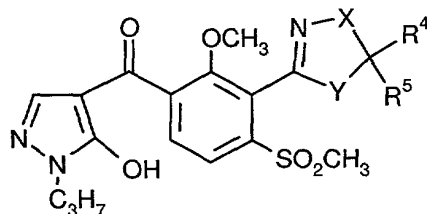
5



- The compounds Ib71.1-Ib71.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

15

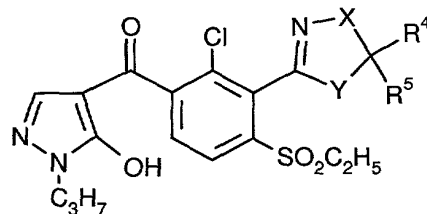
Ib71



- The compounds Ib72.1-Ib72.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

25

Ib72



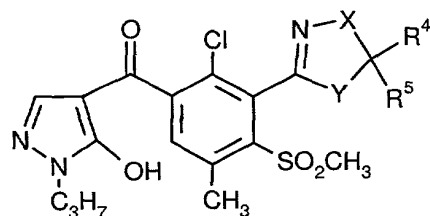
30

- The compounds Ib73.1-Ib73.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is methyl, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

35

Ib73

40



- The compounds Ib74.1-Ib74.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is chlorine, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

45

1b74



- 10



- 20 _



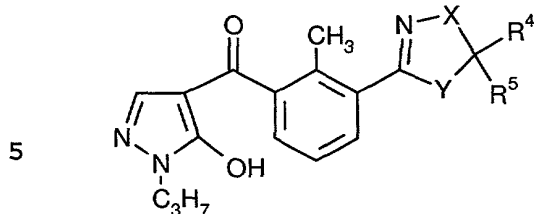
- 35



- 45

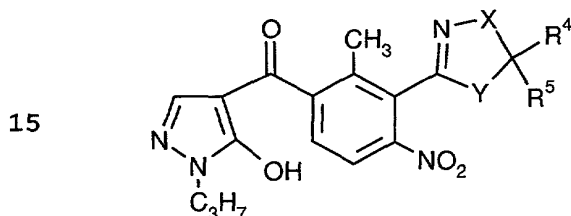
56

Ib78



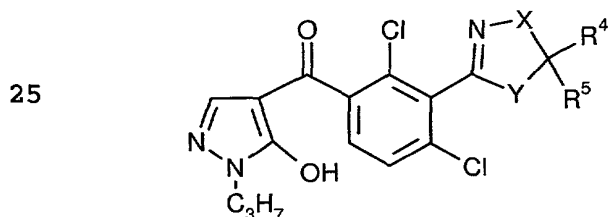
- 10 - The compounds Ib79.1-Ib79.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is nitro, R¹⁶ is n-propyl and R¹⁸ is hydrogen.

Ib79



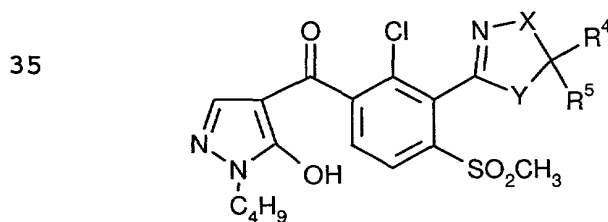
- 20 - The compounds Ib80.1-Ib80.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is n-propyl and R¹⁸ is hydrogen.

Ib80



- 30 - The compounds Ib81.1-Ib81.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib81



- 40 - The compounds Ib82.1-Ib82.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

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57

Chemical structure 57 is a benzimidazole derivative. It features a benzimidazole ring system with a C_4H_9 group at position 2 and a hydroxyl group at position 3. The benzene ring is substituted with a carbonyl group at position 1, a chlorine atom at position 4, and a nitro group (NO_2) at position 5. The carbonyl group is connected to a carbon atom that is also bonded to a nitrogen atom ($\text{N}=\text{X}$) and a carbon atom bonded to two R groups (R^4 and R^5) and a Y group.

57

10

Cc1cc(ccc1C(=O)c2c(O)cnc2C3CCCC3)C(=N)C(Y)C(X)(R4)R5 \mathbb{D}^4

20

CN1C=NC2=C1C(=O)C(=C(C=C2)C(=O)C3=CC=C(C=C3)C(=C(C=C3)C(=O)N(C)C)C(=O)N(C)C)C(=O)N(C)C

35

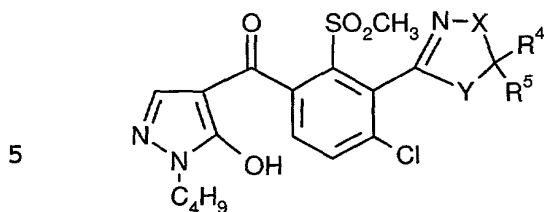
[illegible]

□

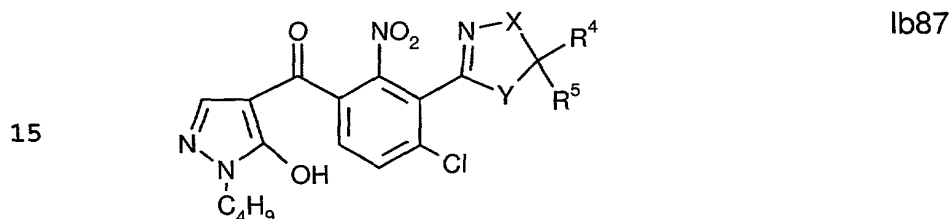
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58

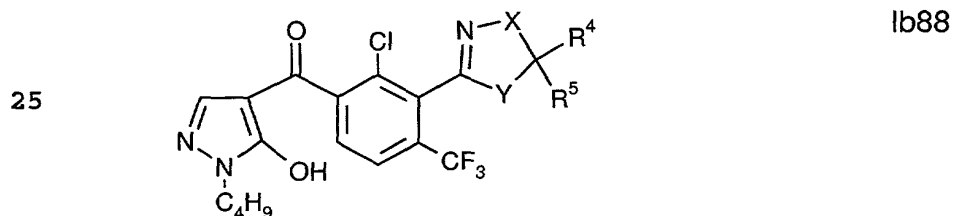
Ib86



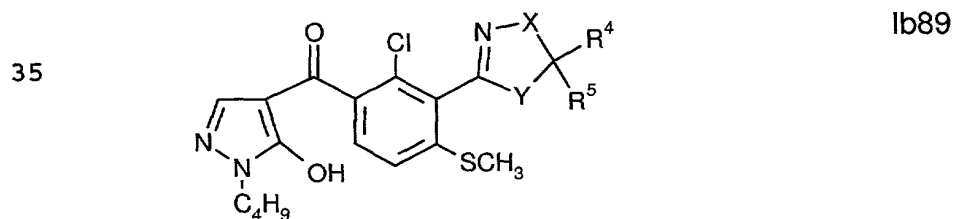
- 10 - The compounds Ib87.1-Ib87.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is n-butyl and R¹⁸ is hydrogen.



- 20 - The compounds Ib88.1-Ib88.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethyl, R¹⁶ is n-butyl and R¹⁸ is hydrogen.



- 30 - The compounds Ib89.1-Ib89.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylthio, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

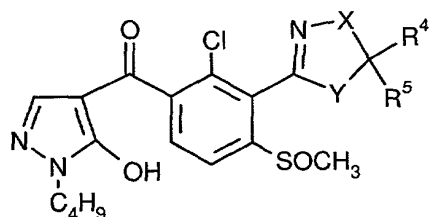


- 40 - The compounds Ib90.1-Ib90.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfinyl, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

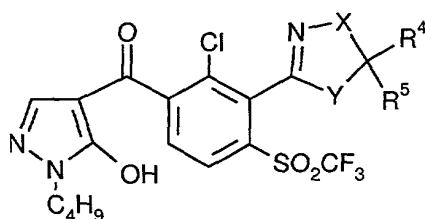
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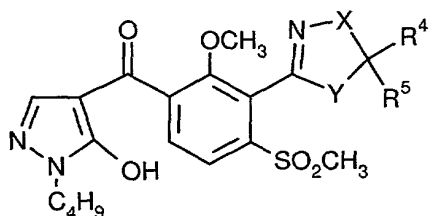
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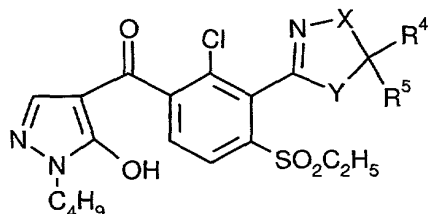
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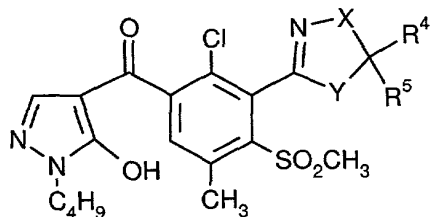


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60

Ib94

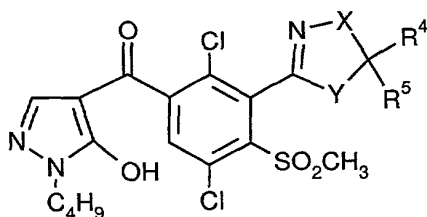
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- 10 - The compounds Ib95.1-Ib95.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is chlorine, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib95

15



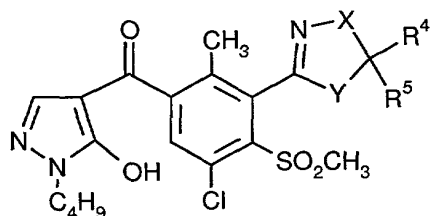
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- 25 - The compounds Ib96.1-Ib96.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is chlorine, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

25

Ib96

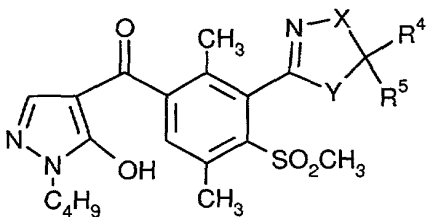
30



- 35 - The compounds Ib97.1-Ib97.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is methyl, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib97

40



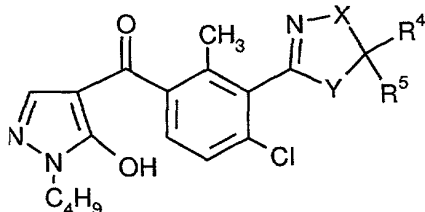
- 45 - The compounds Ib98.1-Ib98.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

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Ib98

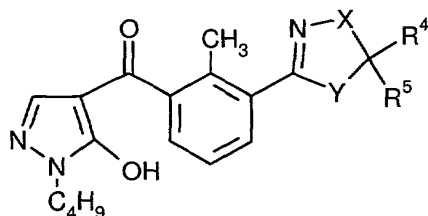
5



- 10 - The compounds Ib99.1-Ib99.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is hydrogen, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib99

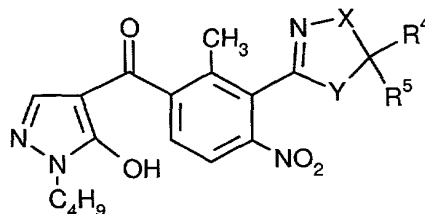
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- 20 - The compounds Ib100.1-Ib100.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is nitro, R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib100

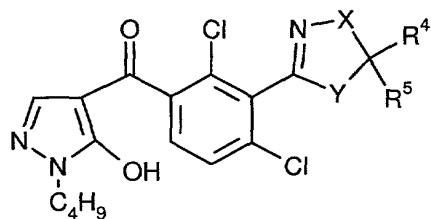
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- 30 - The compounds Ib101.1-Ib101.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is n-butyl and R¹⁸ is hydrogen.

Ib101

35

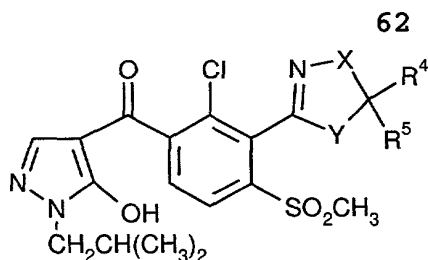


- 40 - The compounds Ib102.1-Ib102.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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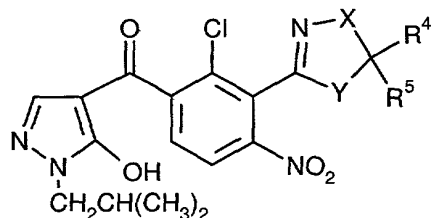
5



Ib102

- The compounds Ib103.1-Ib103.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

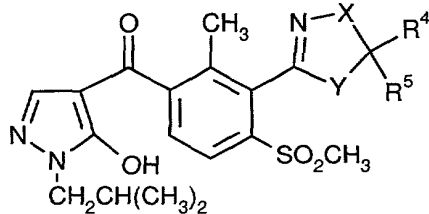
15



Ib103

- The compounds Ib104.1-Ib104.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

25



Ib104

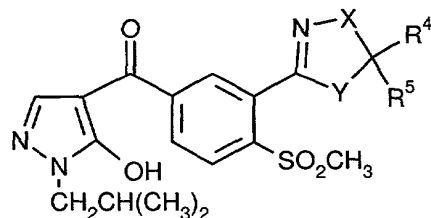
30

- The compounds Ib105.1-Ib105.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is hydrogen, R² is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

35

Ib105

40



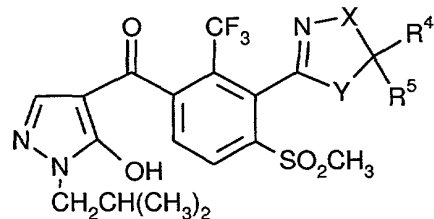
- The compounds Ib106.1-Ib106.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is trifluoromethyl, R² is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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63

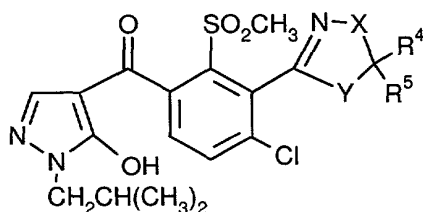
Ib106

5



- 10 - The compounds Ib107.1-Ib107.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

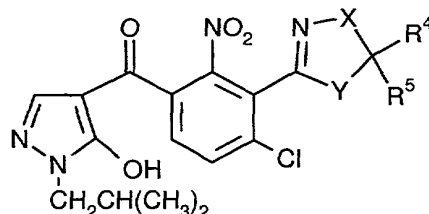
15



Ib107

- 20 - The compounds Ib108.1-Ib108.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

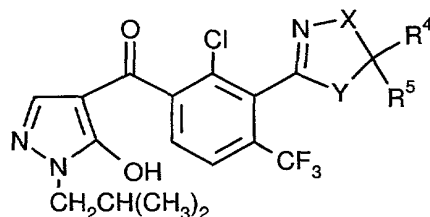
25



Ib108

- 30 - The compounds Ib109.1-Ib109.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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Ib109

- 40 - The compounds Ib110.1-Ib110.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylthio, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

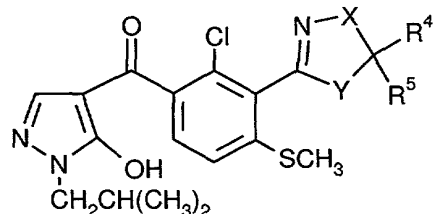
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64

Ib110

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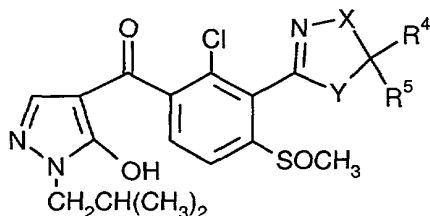


- The compounds Ib111.1-Ib111.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfinyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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Ib111

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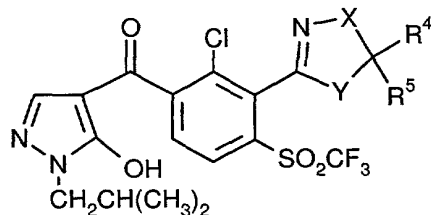


- The compounds Ib112.1-Ib112.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is trifluoromethylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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Ib112

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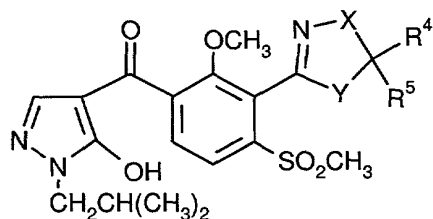


- The compounds Ib113.1-Ib113.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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Ib113

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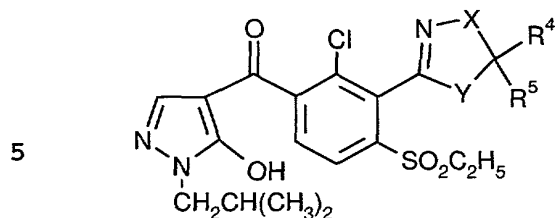
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- The compounds Ib114.1-Ib114.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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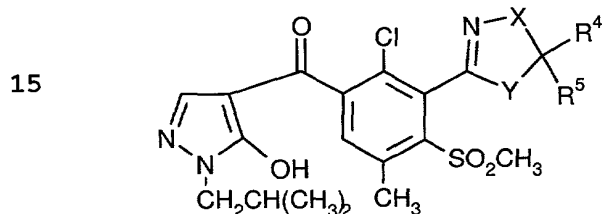
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Ib114



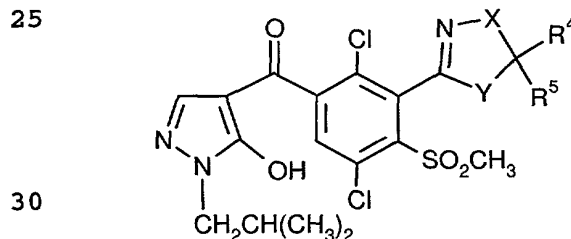
- 10 - The compounds Ib115.1-Ib115.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is methyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

Ib115



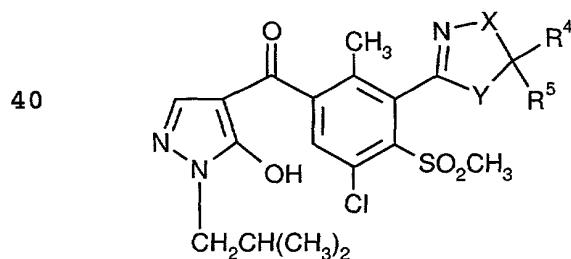
- 20 - The compounds Ib116.1-Ib116.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R³ is chlorine, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

Ib116



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- 35 - The compounds Ib117.1-Ib117.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is chlorine, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

Ib117



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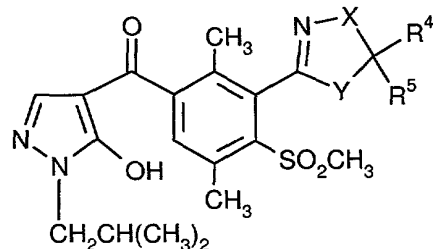
0050/47679-001300-06160

66

- The compounds Ib118.1-Ib118.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R³ is methyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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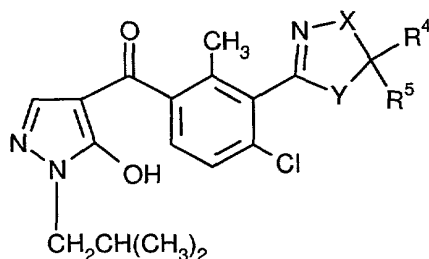


Ib118

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- The compounds Ib119.1-Ib119.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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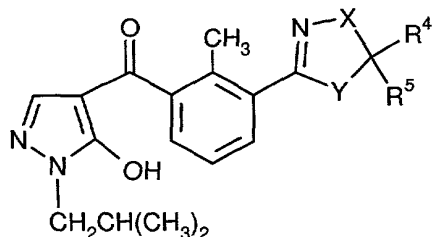


Ib119

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- The compounds Ib120.1-Ib120.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is hydrogen, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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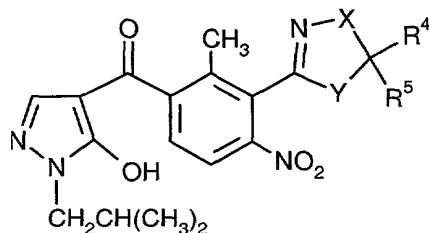


Ib120

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- The compounds Ib121.1-Ib121.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is nitro, R¹⁶ is iso-butyl and R¹⁸ is hydrogen.

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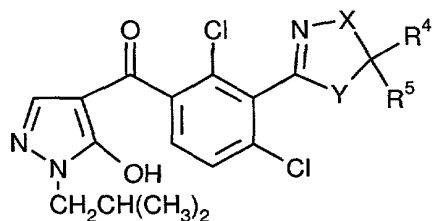


Ib121

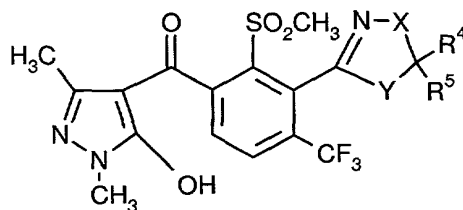
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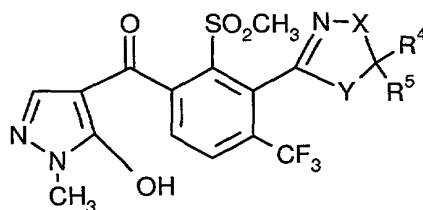
- b122



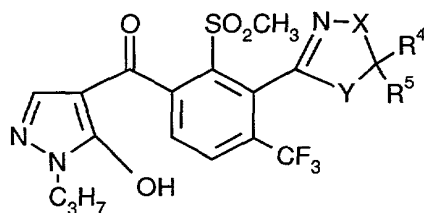
- lb123



- lb124



- lb125



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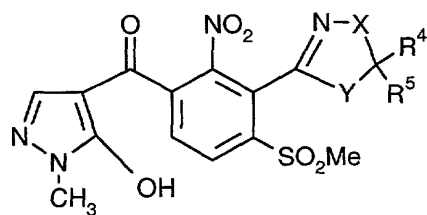


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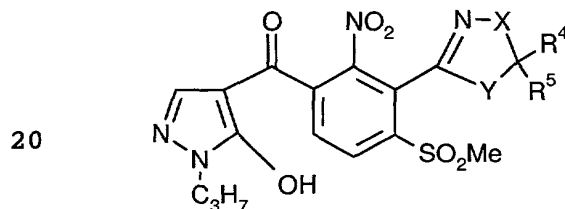
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- lb130



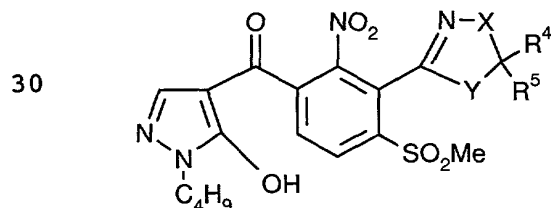
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lb131



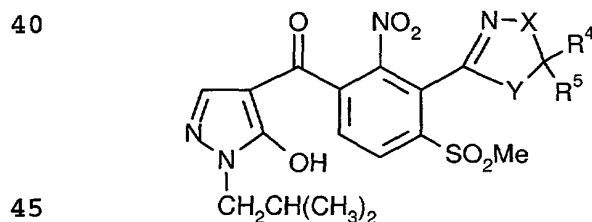
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b1
b3
b7C
b7D



- 35

lb133



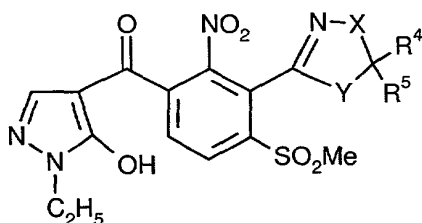
70

- The compounds Ib134.1-Ib134.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R² is methylsulfonyl, R¹⁶ is ethyl and R¹⁸ is hydrogen.

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Ib134

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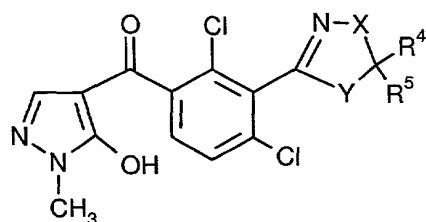


- The compounds Ib135.1-Ib135.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁸ is hydrogen.

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Ib135

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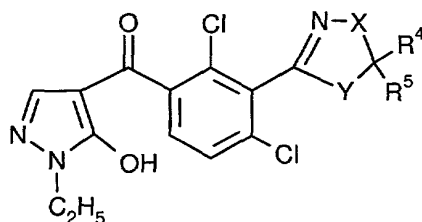


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- The compounds Ib136.1-Ib136.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl and R¹⁸ is hydrogen.

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Ib136

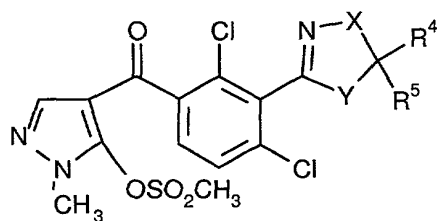


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- The compounds Ib137.1-Ib137.126 which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is methylsulfonyl and R¹⁸ is hydrogen.

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Ib137



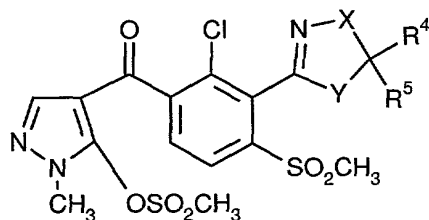
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- The compounds Ib138.1-Ib138.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

71

Ib138

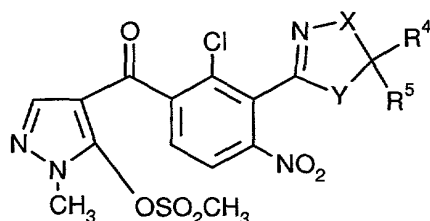
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- 10 - The compounds Ib139.1-Ib139.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, Z is methanesulfonyl and R¹⁸ is hydrogen.

Ib139

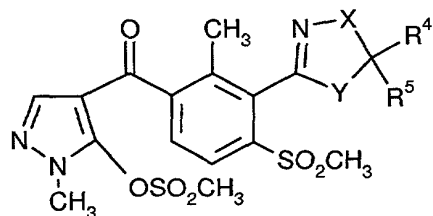
15



- 20 - The compounds Ib140.1-Ib140.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methanesulfonyl, Z is methanesulfonyl and R¹⁸ is hydrogen.

Ib140

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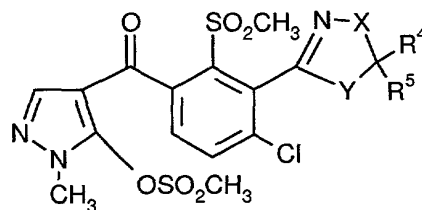


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- The compounds Ib141.1-Ib141.126 which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methanesulfonyl, Z is methanesulfonyl and R¹⁸ is hydrogen.

Ib141

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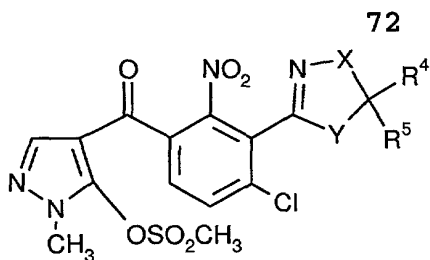
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- The compounds Ib142.1-Ib142.126 which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is methanesulfonyl and R¹⁸ is hydrogen.

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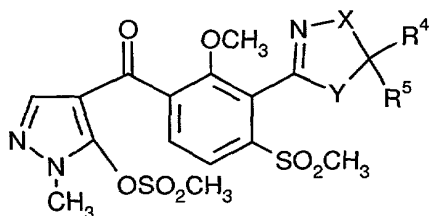
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Ib142

- The compounds Ib143.1-Ib143.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact R¹ is methoxy, R² and Z are methylsulfonyl and R¹⁸ is hydrogen.

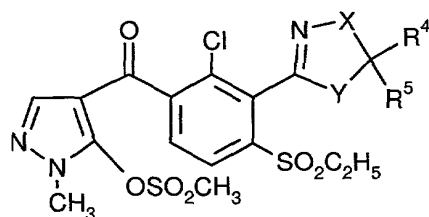
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Ib143

- The compounds Ib144.1-Ib144.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

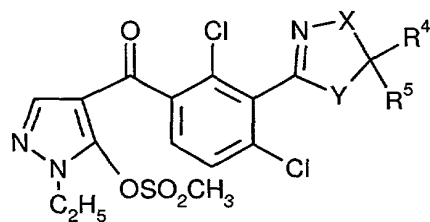
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Ib144

- The compounds Ib145.1-Ib145.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

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Ib145

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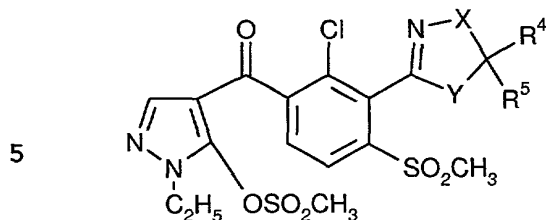
- The compounds Ib146.1-Ib146.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

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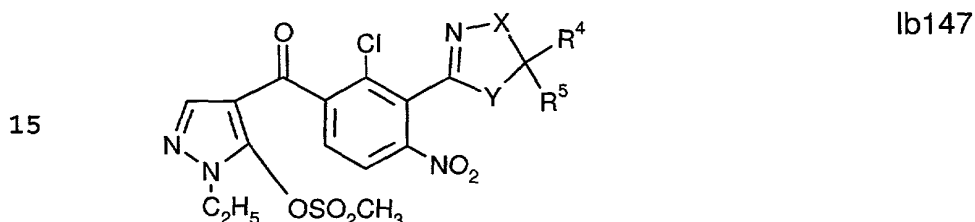
0050/47679-00276060

73

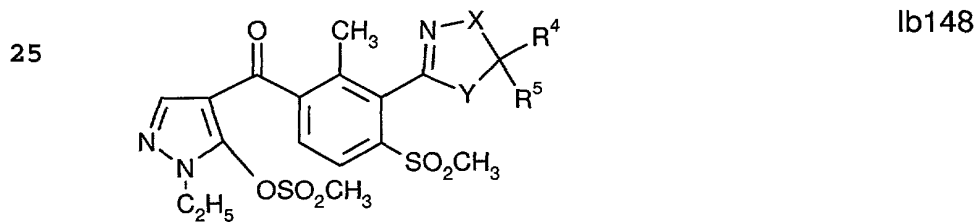
Ib146



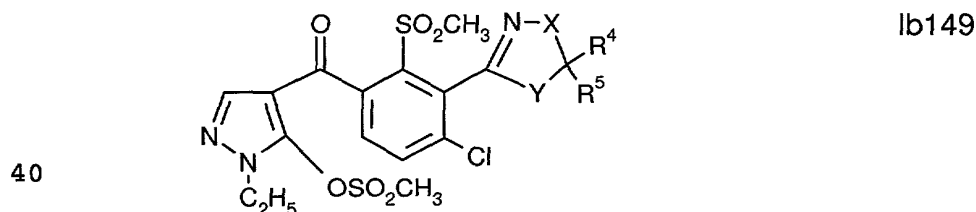
- 10 - The compounds Ib147.1-Ib147.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.



- 20 - The compounds Ib148.1-Ib148.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.



- 30 - The compounds Ib149.1-Ib149.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.



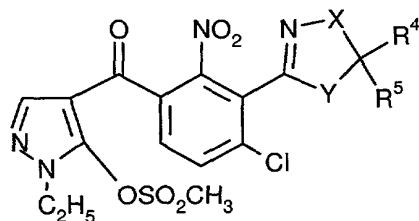
- 40 - The compounds Ib150.1-Ib150.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.
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Ib150

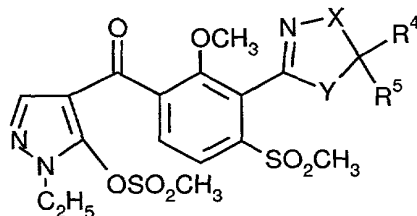
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- The compounds Ib151.1-Ib151.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

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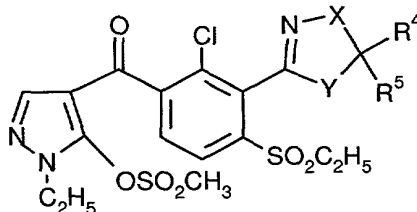
Ib151



- The compounds Ib152.1-Ib152.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is methylsulfonyl and R¹⁸ is hydrogen.

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Ib152

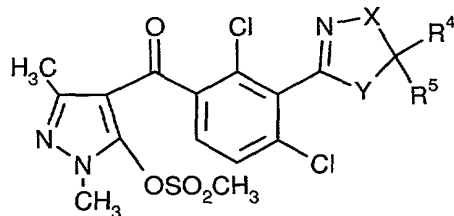


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- The compounds Ib153.1-Ib153.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is methylsulfonyl.

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Ib153



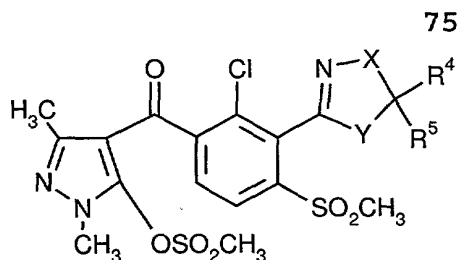
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- The compounds Ib154.1-Ib154.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² and Z are methylsulfonyl.

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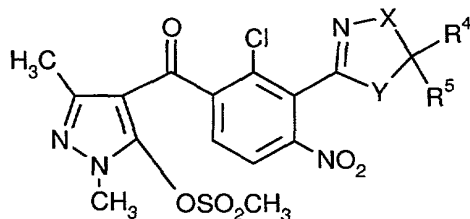


Ib154

10

- The compounds Ib155.1-Ib155.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro and Z is methylsulfonyl.

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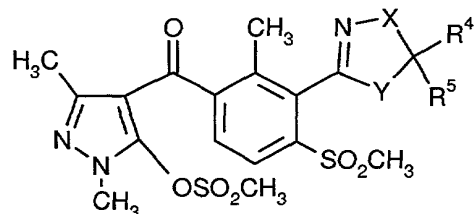


Ib155

20

- The compounds Ib156.1-Ib156.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² and Z are methylsulfonyl.

25

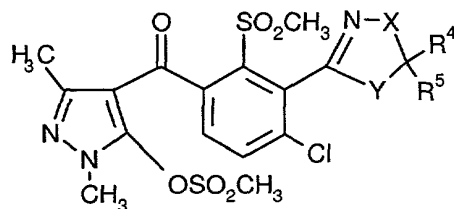


Ib156

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- The compounds Ib157.1-Ib157.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ and Z are methylsulfonyl.

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Ib157

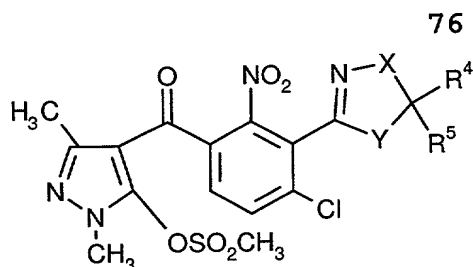
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- The compounds Ib158.1-Ib158.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro and Z is methylsulfonyl.

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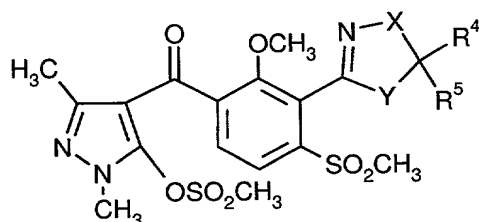
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Ib158

- The compounds Ib159.1-Ib159.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² and Z are methylsulfonyl.

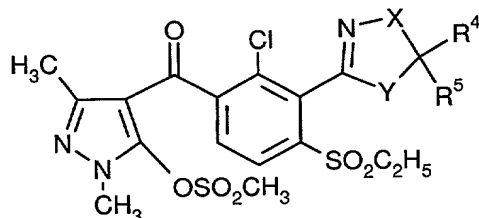
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Ib159

- The compounds Ib160.1-Ib160.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl and Z is methylsulfonyl.

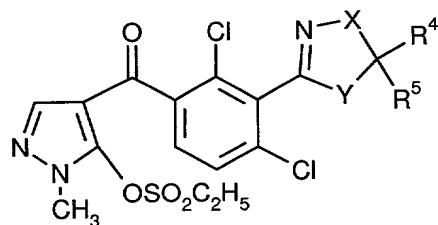
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Ib160

- The compounds Ib161.1-Ib161.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is ethylsulfonyl and R¹⁸ is hydrogen.

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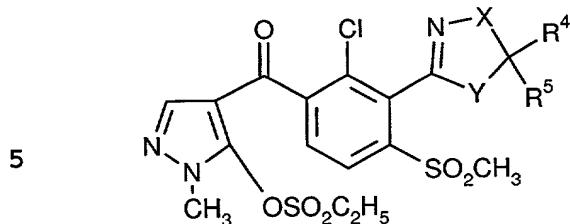
Ib161

- The compounds Ib162.1-Ib162.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.

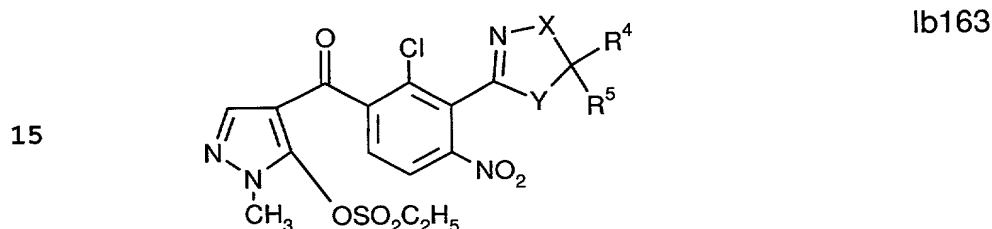
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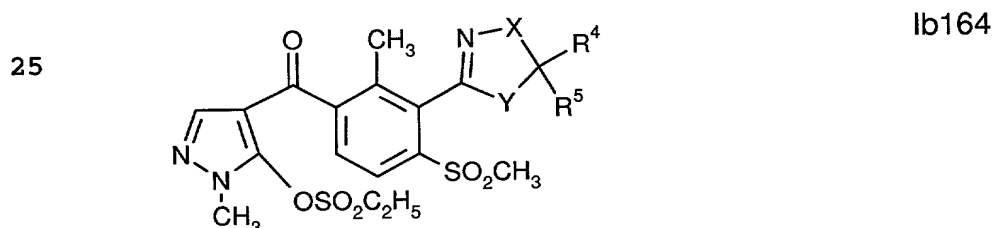
Ib162



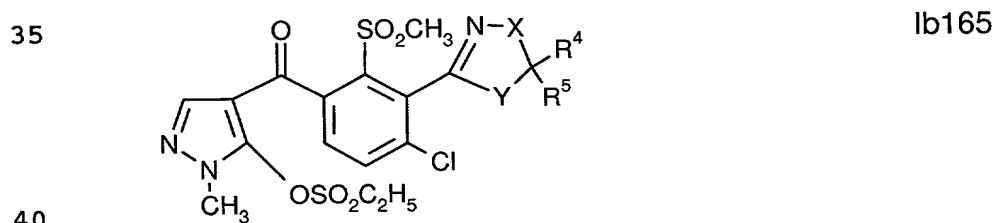
- 10 - The compounds Ib163.1-Ib163.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, Z is ethylsulfonyl and R¹⁸ is hydrogen.



- 20 - The compounds Ib164.1-Ib164.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.



- 30 - The compounds Ib165.1-Ib165.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.



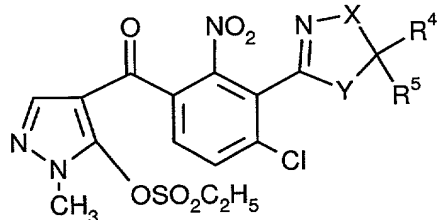
- 45 - The compounds Ib166.1-Ib166.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is ethylsulfonyl and R¹⁸ is hydrogen.

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Ib166

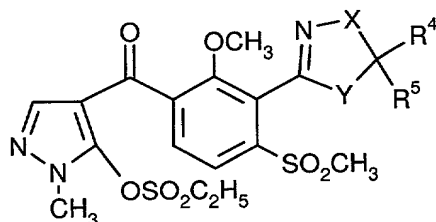
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- The compounds Ib167.1-Ib167.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.

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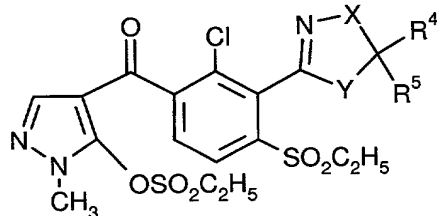


Ib167

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- The compounds Ib168.1-Ib168.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² and Z are ethylsulfonyl and R¹⁸ is hydrogen.

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Ib168

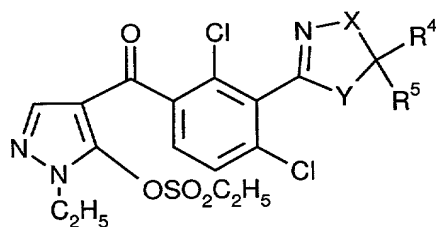
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- The compounds Ib169.1-Ib169.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.

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Ib169

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- The compounds Ib170.1-Ib170.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is ethylsulfonyl and R¹⁸ is hydrogen.

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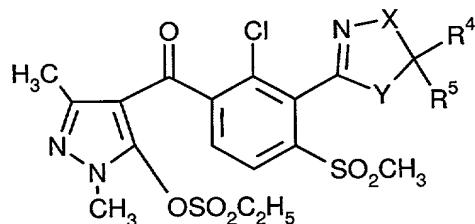
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Ib178

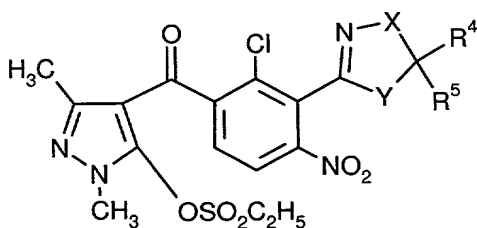
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- 10 - The compounds Ib179.1-Ib179.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro and Z is ethylsulfonyl.

Ib179

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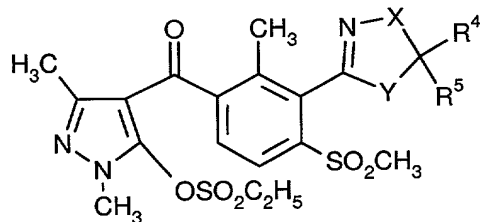


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- The compounds Ib180.1-Ib180.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl and Z is ethylsulfonyl.

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Ib180

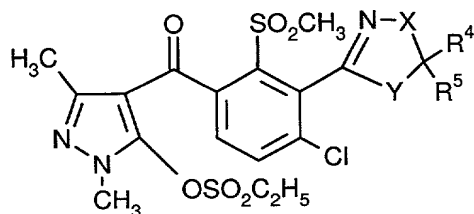


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- The compounds Ib181.1-Ib181.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl and Z is ethylsulfonyl.

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Ib181



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- The compounds Ib182.1-Ib182.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro and Z is ethylsulfonyl.

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82

Chemical structure 82 is a pyrazole derivative. It features a pyrazole ring substituted with a methyl group (H_3C) at position 3, a methyl group (CH_3) at position 4, and a carbonyl group ($\text{C}=\text{O}$) at position 5. The carbonyl group is linked to a benzene ring at position 1. The benzene ring has a nitro group (NO_2) at position 2, a chlorine atom (Cl) at position 3, and a sulfonamide group ($\text{OSO}_2\text{C}_2\text{H}_5$) at position 4. The benzene ring is also linked to a pyrazole ring at position 5. The pyrazole ring has a substituent X at position 3 and a substituent Y at position 4. The pyrazole ring is also linked to a quaternary carbon atom at position 5, which is bonded to R^4 and R^5 .

82

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Cc1nc2c(c1)c(C(=O)c3cc(OC)c(C(=N)C4(C)C4)cc3C(=O)OCC)c(C2)c3ccccc3

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CN1C=NC2=C1C(=O)C(=O)c3cc(Cl)c(C=N[C@@](R4)(R5)Y)c(S(=O)(=O)CC)c3

30 -

CN1C=NC2=C1C(=O)C(=C2)C(=O)c3cc(Cl)c(C(=NXC)(Y)R4)cc3ClOS(=O)(=O)CC

40

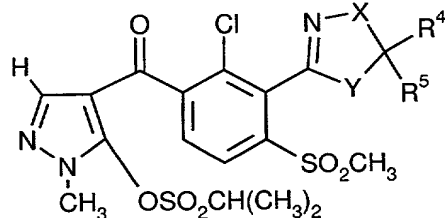
-

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83

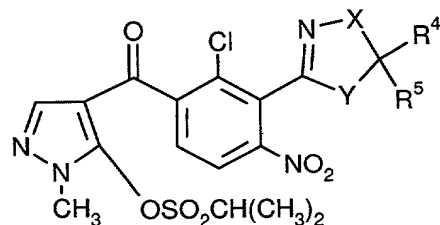
Ib186

5



- The compounds Ib187.1-Ib187.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

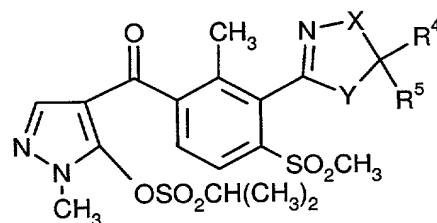
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Ib187

- The compounds Ib188.1-Ib188.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

25

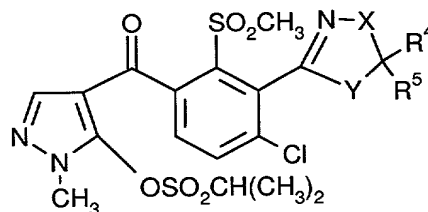


Ib188

30

- The compounds Ib189.1-Ib189.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

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Ib189

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- The compounds Ib190.1-Ib190.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

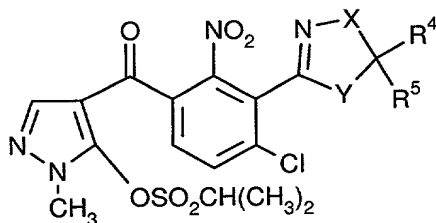
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84

Ib190

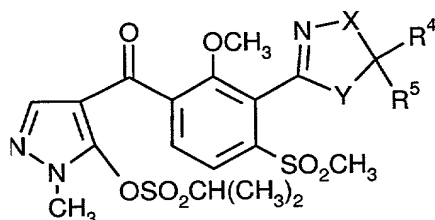
5



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- The compounds Ib191.1-Ib191.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

15

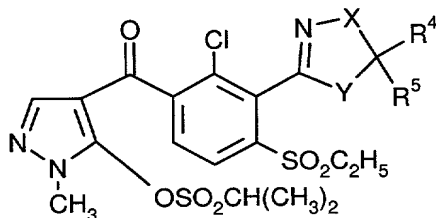


Ib191

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- The compounds Ib192.1-Ib192.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

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Ib192

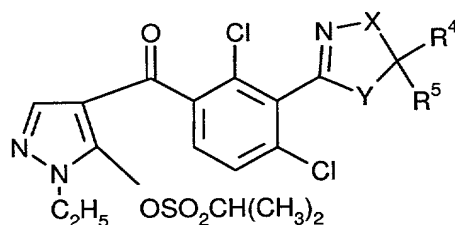
30

- The compounds Ib193.1-Ib193.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

35

Ib193

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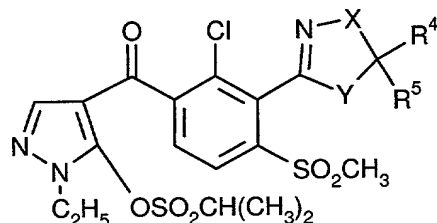
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- The compounds Ib194.1-Ib194.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

85

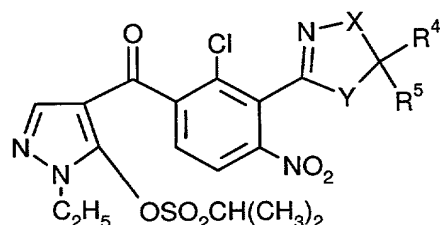
Ib194

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- 10 - The compounds Ib195.1-Ib195.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

15

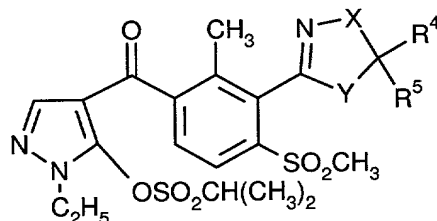


Ib195

20 -

- The compounds Ib196.1-Ib196.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

25

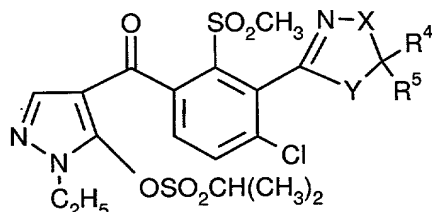


Ib196

30

- 35 - The compounds Ib197.1-Ib197.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

40

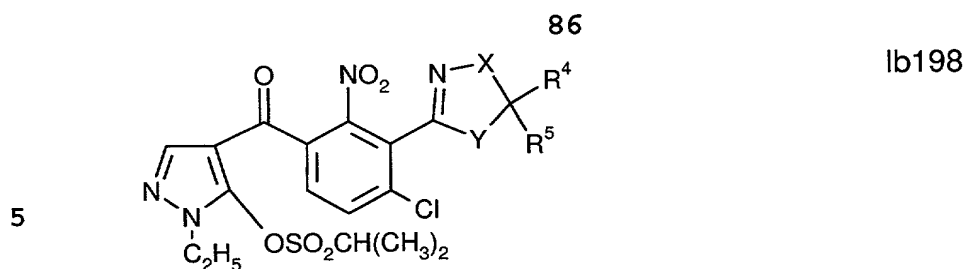


Ib197

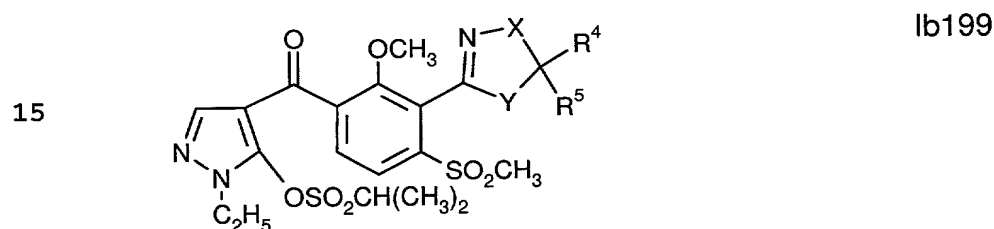
45

- The compounds Ib198.1-Ib198.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.

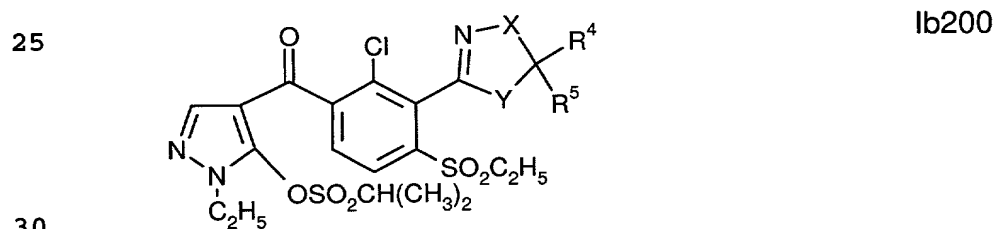
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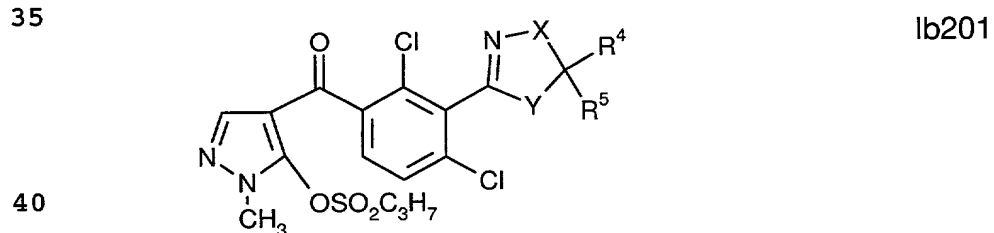
- 10 - The compounds Ib199.1-Ib199.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.



- 20 - The compounds Ib200.1-Ib200.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is iso-propylsulfonyl and R¹⁸ is hydrogen.



- 35 - The compounds Ib201.1-Ib201.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is n-propylsulfonyl and R¹⁸ is hydrogen.

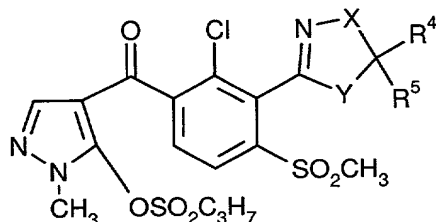


- 45 - The compounds Ib202.1-Ib202.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

87

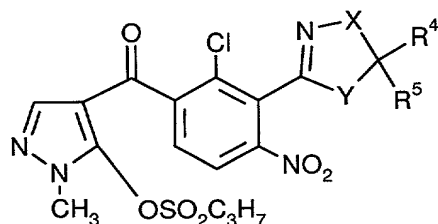
Ib202

5



- The compounds Ib203.1-Ib203.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

15

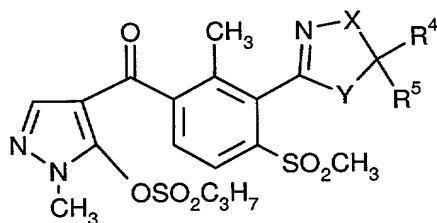


Ib203

20

- The compounds Ib204.1-Ib204.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

25

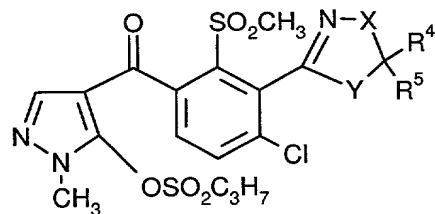


Ib204

30

- The compounds Ib205.1-Ib205.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

35



Ib205

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- The compounds Ib206.1-Ib206.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

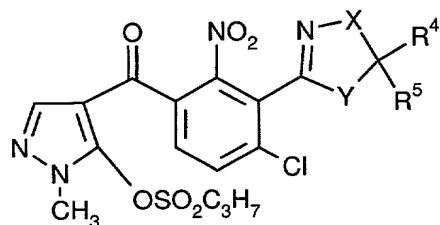
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Ib206

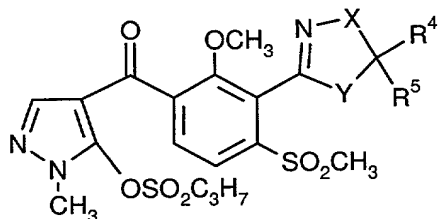
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- The compounds Ib207.1-Ib207.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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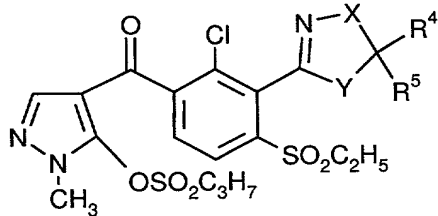


Ib207

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- The compounds Ib.208.1-Ib208.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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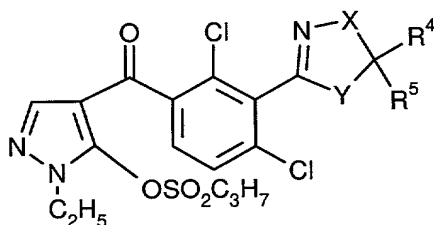


Ib208

30

- The compounds Ib209.1-Ib209.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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Ib209

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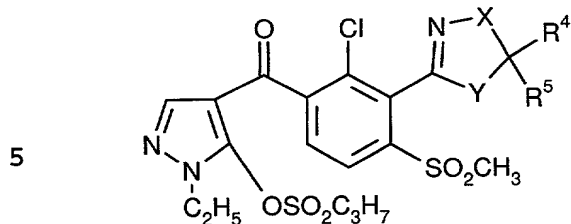
- The compounds Ib210.1-Ib210.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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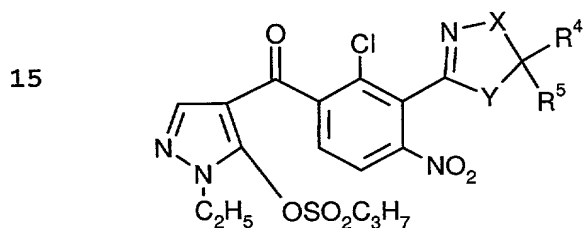
89

Ib210



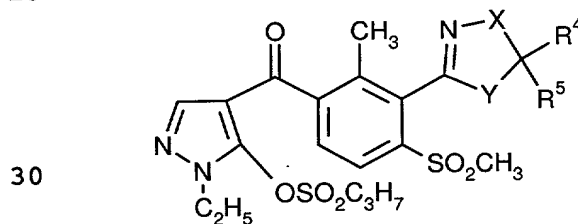
- 10 - The compounds Ib211.1-211.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^2 is nitro, R^{16} is ethyl, Z is n-propylsulfonyl and R^{18} is hydrogen.

Ib211



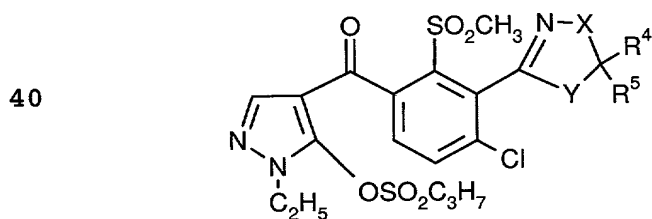
- 20 - The compounds Ib212.1-Ib212.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^1 is methyl, R^2 is methylsulfonyl, R^{16} is ethyl, Z is n-propylsulfonyl and R^{18} is hydrogen.

Ib212



- 35 - The compounds Ib213.1-Ib213.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R^1 is methylsulfonyl, R^{16} is ethyl, Z is n-propylsulfonyl and R^{18} is hydrogen.

Ib213



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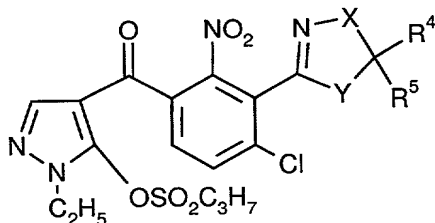
90

- The compounds Ib214.1-Ib214.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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Ib214

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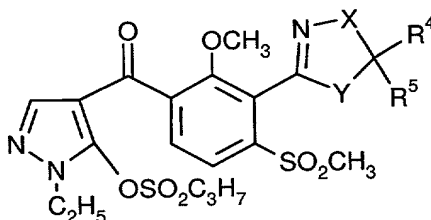


15

- The compounds Ib215.1-Ib215.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is ethyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

20

Ib215

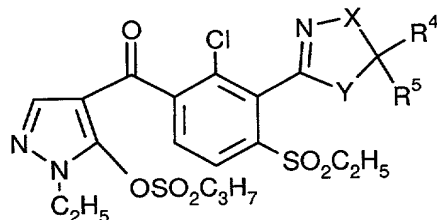


25

- The compounds Ib216.1-Ib216.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is n-propylsulfonyl and R¹⁸ is hydrogen.

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Ib216



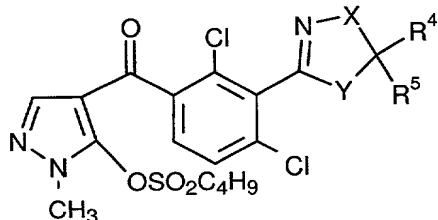
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- The compounds Ib217.1-Ib217.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is n-butylsulfonyl and R¹⁸ is hydrogen.

40

Ib217

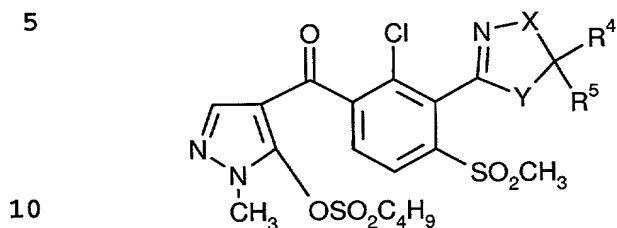
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91

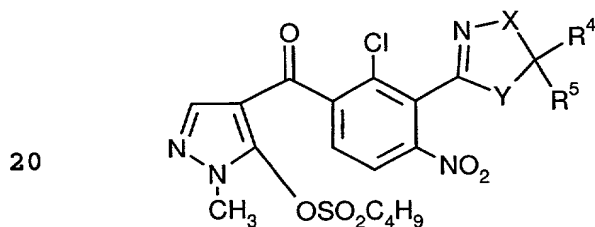
- The compounds Ib218.1-Ib218.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

Ib218



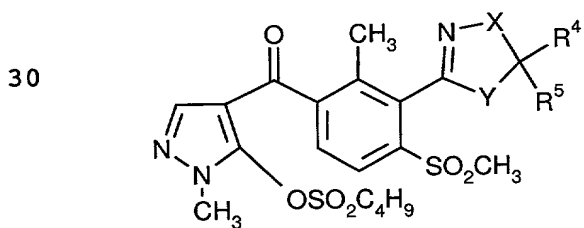
- The compounds Ib219.1-Ib219.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

Ib 219



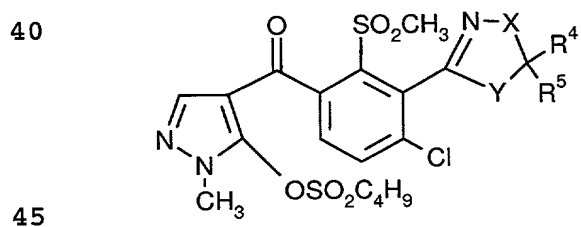
- The compounds Ib220.1-Ib220.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

Ib220



- 35
- The compounds Ib221.1-Ib221.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

Ib221



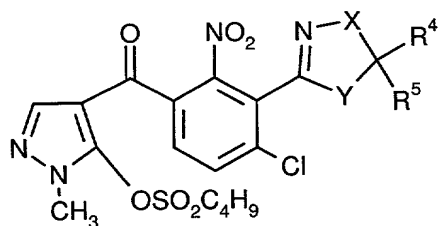
92

- The compounds Ib222.1-Ib222.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

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Ib222

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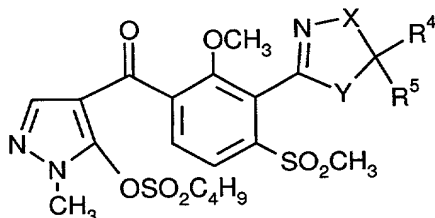


15

- The compounds Ib223.1-Ib223.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

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Ib223

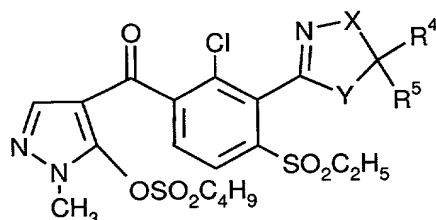


25

- The compounds Ib224.1-Ib224.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

30

Ib224

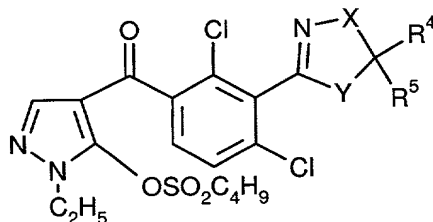


35

- The compounds Ib225.1-Ib225.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

40

Ib225



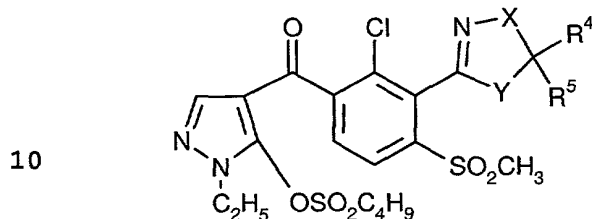
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93

- The compounds Ib226.1-Ib226.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

5

Ib226

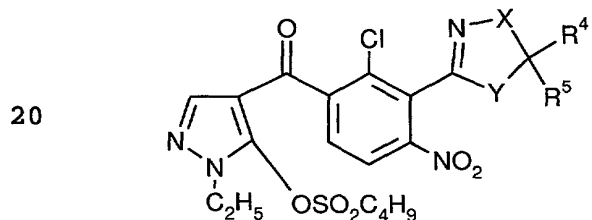


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- The compounds Ib227.1-Ib227.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

15

Ib227

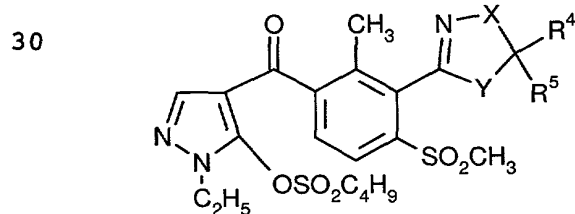


20

- The compounds Ib228.1-Ib228.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

25

Ib228



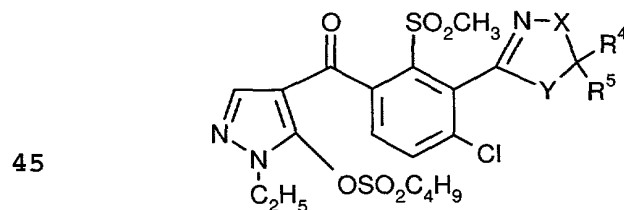
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35

- The compounds Ib229.1-Ib229.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

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Ib229



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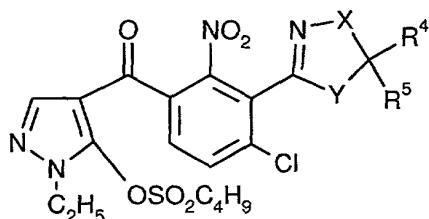
94

- The compounds Ib230.1-Ib230.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

5

Ib230

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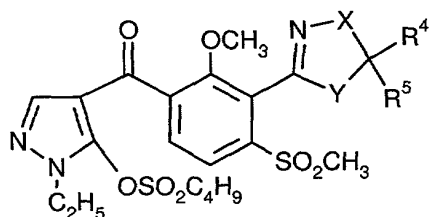


15

- The compounds Ib231.1-Ib231.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

20

Ib231



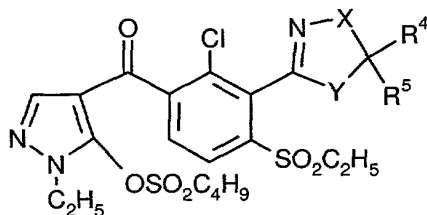
25

- The compounds Ib232.1-Ib232.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is n-butylsulfonyl and R¹⁸ is hydrogen.

30

Ib232

35

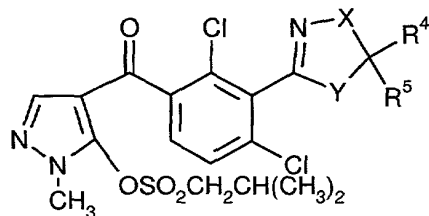


40

- The compounds Ib233.1-Ib233.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

45

Ib233



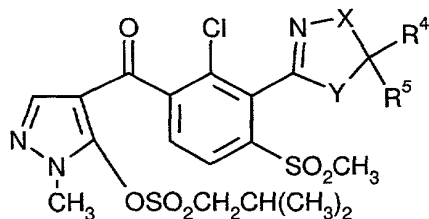
95

- The compounds Ib234.1-Ib234.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

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Ib234

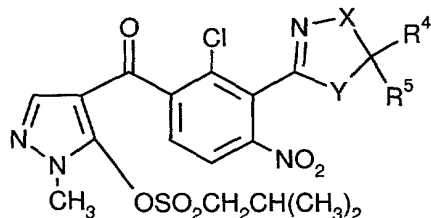
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15

Ib235

20

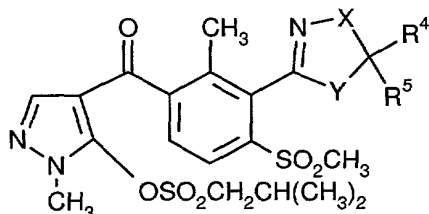


25

- The compounds Ib236.1-Ib236.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

30

Ib236

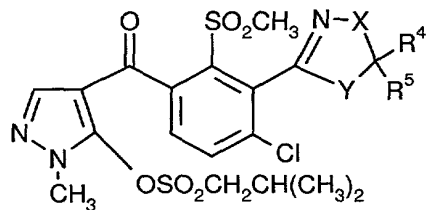


35

- The compounds Ib237.1-Ib237.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

40

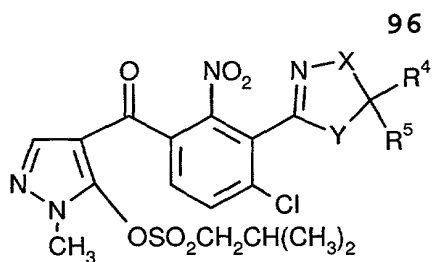
Ib237



45

- The compounds Ib238.1-Ib238.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

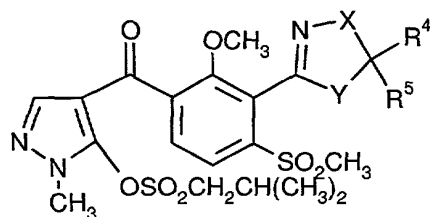
5



Ib238

- The compounds Ib239.1-Ib239.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methoxy, R² is methylsulfonyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

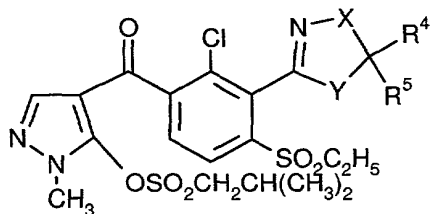
15



Ib239

- The compounds Ib240.1-Ib240.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

25

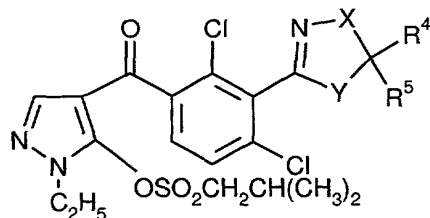


Ib240

30

- The compounds Ib241.1-Ib241.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

35



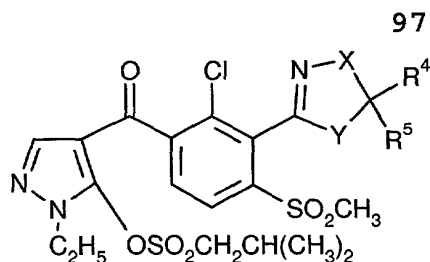
Ib241

40

- The compounds Ib242.1-Ib242.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

45

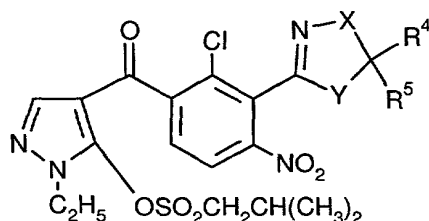
5



Ib242

- The compounds Ib243.1-Ib243.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is nitro, R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

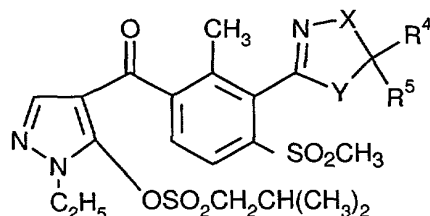
15



Ib243

- The compounds Ib244.1-Ib244.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

25



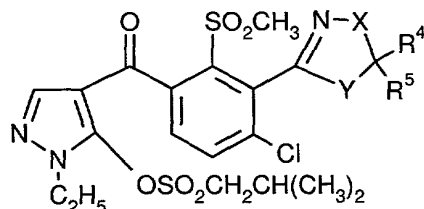
Ib244

30

- The compounds Ib245.1-Ib245.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methylsulfonyl, R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

35

40



Ib245

- The compounds Ib246.1-Ib246.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is nitro, R¹⁶ is ethyl, Z is iso-butylsulfonyl and R¹⁸ is hydrogen.

45



- 10



- 20



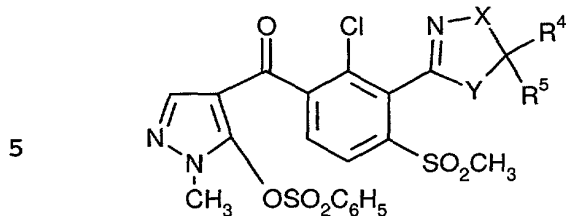
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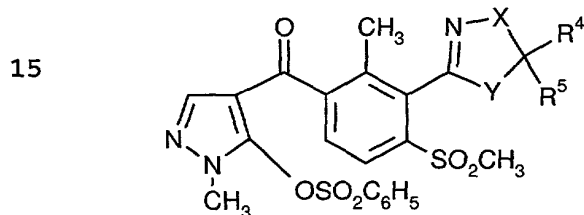
99

Ib250



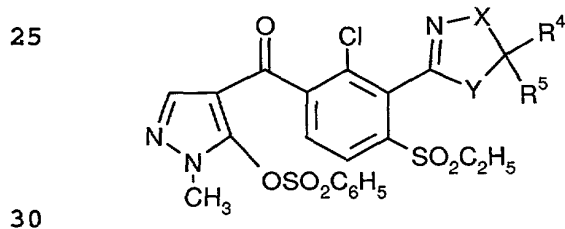
- 10 - The compounds Ib251.1-Ib251.126 which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.

Ib251



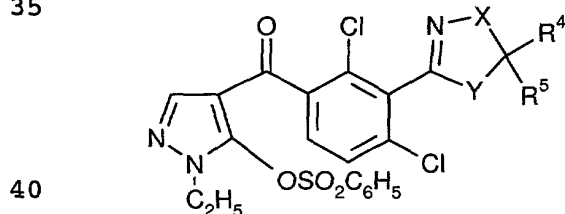
- 20 - The compounds Ib252.1-Ib252.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.

Ib252



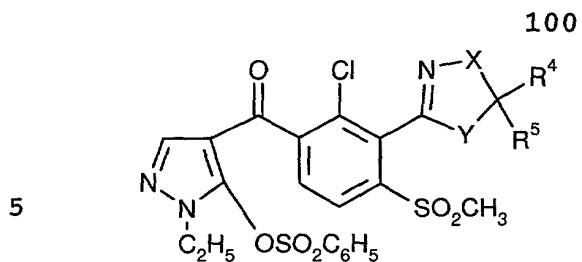
- 35 - The compounds Ib253.1-Ib253.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.

Ib253



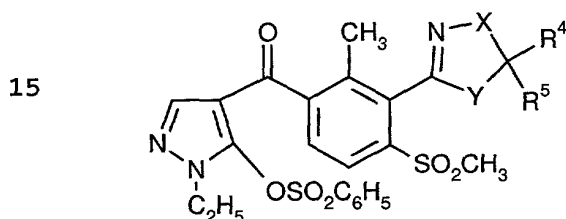
- 45 - The compounds Ib254.1-Ib254.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.

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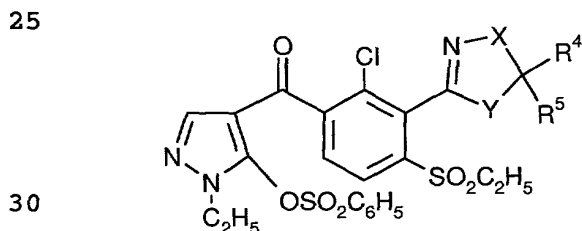
Ib254

- The compounds Ib255.1-Ib255.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.



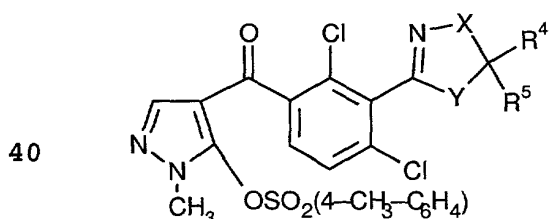
Ib255

- The compounds Ib256.1-Ib256.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is phenylsulfonyl and R¹⁸ is hydrogen.



Ib256

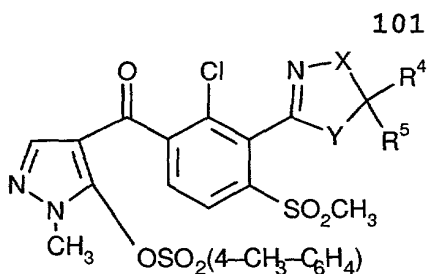
- The compounds Ib257.1-Ib257.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that Z is p-toluenesulfonyl and R¹⁸ is hydrogen.



Ib257

- The compounds Ib258.1-Ib258.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

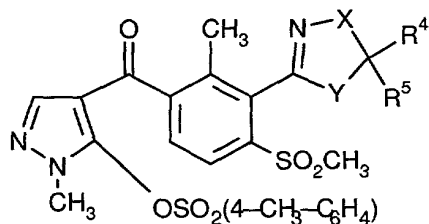
5



Ib258

- The compounds Ib259.1-Ib259.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

15

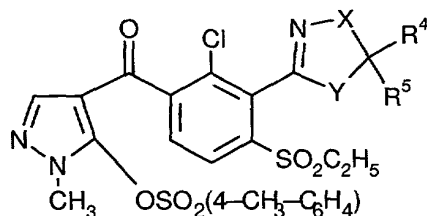


Ib259

20

- The compounds Ib260.1-Ib260.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

25

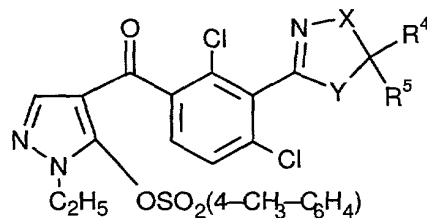


Ib260

30

- The compounds Ib261.1-Ib261.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹⁶ is ethyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

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Ib261

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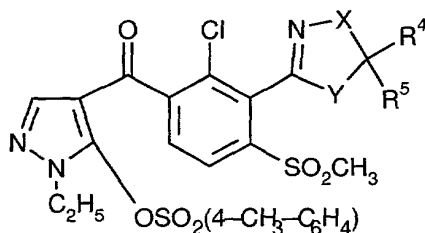
102

- The compounds Ib262.1-Ib262.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is methylsulfonyl, R¹⁶ is ethyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

5

Ib262

10

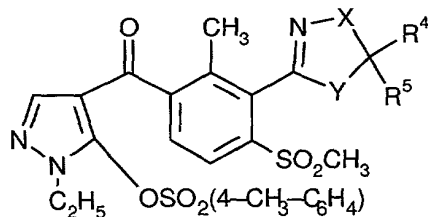


15

- The compounds Ib263.1-Ib263.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R¹ is methyl, R² is methylsulfonyl, R¹⁶ is ethyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

20

Ib263



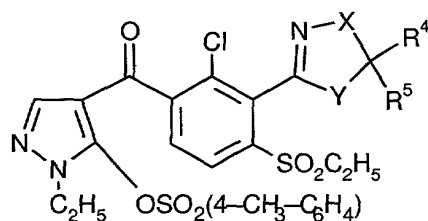
25

- The compounds Ib264-Ib264.126, which differ from the corresponding compounds Ib1.1-Ib1.126 by the fact that R² is ethylsulfonyl, R¹⁶ is ethyl, Z is p-toluenesulfonyl and R¹⁸ is hydrogen.

30

Ib264

35



Also particularly preferred are 3-heterocyclyl-substituted benzoyl derivatives of the formula I where:

40

- R¹ is halogen, C₁-C₆-alkyl, C₁-C₆-alkylthio or C₁-C₆-alkylsulfonyl;
in particular chlorine, methyl, methylthio or methylsulfonyl;

45

- R² is hydrogen, nitro, halogen, C₁-C₆-alkylthio, C₁-C₆-alkylsulfinyl or C₁-C₆-alkylsulfonyl;

103

in particular hydrogen, nitro, chlorine, methylthio, methylsulfinyl, methylsulfonyl, ethylsulfonyl or propylsulfonyl;

5 R³ is hydrogen;

R⁴, R⁵ are hydrogen, halogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy, C₁-C₄-alkylthio or COR⁶;
 10 in particular hydrogen, fluorine, methyl, ethyl, propyl, trifluoromethyl, chloromethyl, 1-chloroeth-1-yl, methoxy, ethoxy, ethylthio or ethoxycarbonyl;

or

15 R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to polysubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

20 R⁶ is C₁-C₄-alkoxy;
 in particular ethyl;

X is O or CR¹⁰R¹¹;

25 Y is O, S or CR¹³R¹⁴;

R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl or C₁-C₄-haloalkyl; in particular hydrogen, methyl or chloromethyl;

30 or

R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to polysubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is
 35 unsubstituted or substituted by C₁-C₄-alkyl;
 in particular 1,3-propanediyl;

R¹⁶ is C₁-C₆-alkyl;
 in particular methyl, ethyl, propyl, 2-methylpropyl or
 40 butyl;

Z is H or SO₂R¹⁷;

R¹⁷ is C₁-C₄-alkyl;
 45 in particular methyl, ethyl, propyl or 2-methylpropyl;

104

with the exception of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-ethyl-5-hydroxy-1H-pyrazole, 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole, 4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;

10 and the agriculturally useful salts thereof;
in particular alkali metal salts and ammonium salts.

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The 3-heterocyclyl-substituted benzoyl derivatives of the formula I are obtainable by various routes, for example by the following process:

5

Process A:

Reaction of pyrazoles of the formula II (where Z = H) with an
10 activated benzoic acid III α or a benzoic acid III β , which is preferably activated in situ to give the acylating product and subsequently subjecting the latter to a rearrangement reaction.

15

20

25

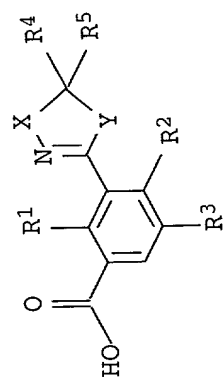
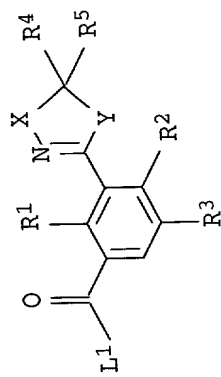
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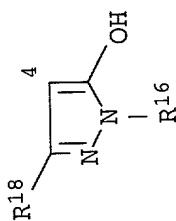
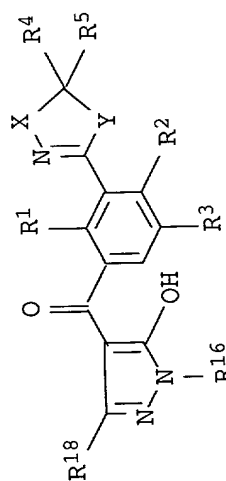
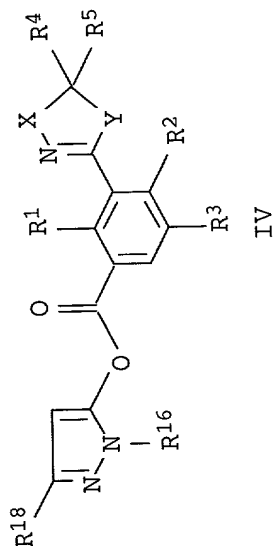
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III β 

+

II (where $Z = \text{H}$)III α I (where $Z = \text{H}$)

IV

L¹ is a nucleophilically displaceable leaving group such as halogen, eg. bromine, chlorine, hetaryl, eg. imidazolyl, pyridyl, carboxylate, eg. acetate, trifluoroacetate, and the like.

5

The activated benzoic acid can be employed directly, as in the case of the benzoyl halides, or it can be prepared in situ, for example with dicyclohexylcarbodiimide, triphenylphosphine/azodicarboxylic ester, 2-pyridine disulfide/triphenylphosphine, carbonyldiimidazole and the like.

10

It may be advantageous to carry out the acylation reaction in the presence of a base. The reactants and the auxiliary base are expediently employed in equimolar amounts. A small excess of the auxiliary base, for example 1.2 to 1.5 mol equivalents based on II, may be advantageous under certain circumstances.

15

Suitable auxiliary bases are tertiary alkylamines, pyridine or alkali metal carbonates. Examples of solvents which can be used are chlorinated hydrocarbons such as methylene chloride, 1,2-dichloroethane, aromatic hydrocarbons such as toluene, xylene, chlorobenzene, ethers such as diethyl ether, methyl tert-butyl ether, tetrahydrofuran, dioxane, polar aprotic solvents such as acetonitrile, dimethylformamide, dimethyl sulfoxide, or esters such as ethyl acetate, or mixtures of these.

20

25

If benzoyl halides are employed as activated carboxylic acid component, it may be expedient to cool the reaction mixture to 0-10°C when adding this reactant. The mixture is subsequently stirred at 20 - 100°C, preferably at 25 - 50°C, until the reaction is complete. Work-up is carried out in the customary manner, for example the reaction mixture is poured into water and the product of value is extracted. Especially suitable solvents for this purpose are methylene chloride, diethyl ether and ethyl acetate. After the organic phase has been dried and the solvent removed, the crude ester can be employed without further purification for the rearrangement reaction.

30

35

Rearrangement of the esters to give the compounds of the formula I is expediently carried out at from 20 to 40°C in a solvent and in the presence of a base and, if appropriate, with the aid of a cyano compound as catalyst.

40

45

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Examples of solvents which can be used are acetonitrile, methylene chloride, 1,2-dichlorethane, dioxane, ethyl acetate, toluene or mixtures of these. Preferred solvents are acetonitrile and dioxane.

5

Suitable bases are tertiary amines such triethylamine, pyridine, or alkali metal carbonates such as sodium carbonate, potassium carbonate, all of which are preferably employed in equimolar amounts or up to a fourfold excess, based on the ester.

10 Triethylamine or alkali metal carbonate are preferably used, but by preference in a ratio of twice the equimolar amount based on the ester.

15 Suitable cyano compounds are inorganic cyanides such as sodium cyanide, potassium cyanide, and organic cyano compounds such as acetone cyanohydrin, trimethylsilyl cyanide. They are employed in an amount of from 1 to 50 mol percent, based on the ester. Substances which are preferably employed are acetone cyanohydrin or trimethylsilyl cyanide, for example in an amount of from 5 to
20 15, preferably 10, mol percent, based on the ester.

Work-up can be effected in a manner known per se. For example, the reaction mixture is acidified with dilute mineral acid, such
25 as 5% strength hydrochloric acid or sulfuric acid, and extracted with an organic solvent, eg. methylene chloride or ethyl acetate. The organic extract can be extracted with 5-10% strength alkali metal carbonate solution, eg. sodium carbonate or potassium carbonate solution. The aqueous phase is acidified, and the
30 precipitate which forms is filtered off with suction and/or extracted with methylene chloride or ethyl acetate, dried and concentrated.

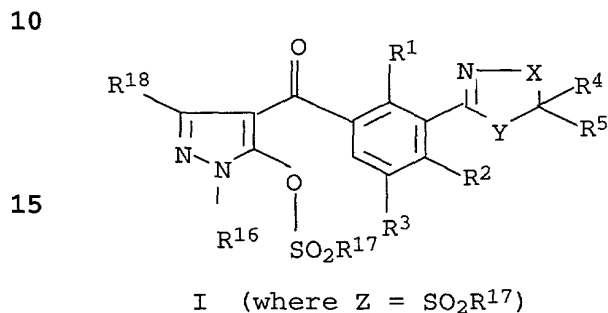
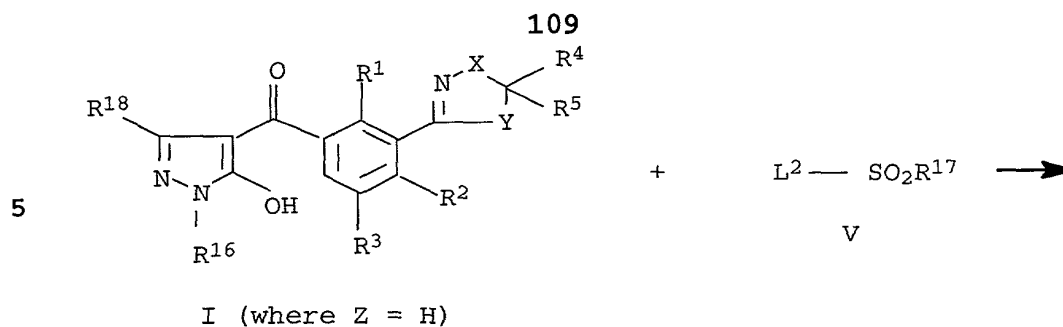
(Examples of the synthesis of esters from hydroxypyrazoles and of the rearrangement of the esters are mentioned, for example, in
35 EP-A 282 944 and US 4 643 757).

Process B:

40 Reaction of 3-heterocycllyl-substituted benzoyl derivatives of the formula I (where Z = H) with a compound of the formula V (where Z = SO₂R¹⁷):

45

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- 20 L² is a nucleophilically displaceable leaving group, such as halogen, eg. bromine, chlorine, hetaryl, eg. imidazolyl, pyridyl, sulfonate, eg. OSO₂R¹⁷.
- 25 The compounds of the formula V can be employed directly such as, for example, in the case of the sulfonyl halides or sulfonic anhydrides, or they can be prepared in situ, for example activated sulfonic acids (by means of sulfonic acid and dicyclohexylcarbodiimide, carbonyldiimidazole and the like).
- 30 As a rule, the starting compounds are employed in an equimolar ratio. However, it may also be advantageous to employ an excess of one or the other component.
- 35 It may be advantageous to carry out the reaction in the presence of a base. The reactants and the auxiliary base are expediently employed in equimolar ratios. An excess of the auxiliary base, for example 1.5 to 3 mol equivalents, based on II, may be advantageous under certain circumstances.
- 40 Suitable auxiliary bases are tertiary alkylamines such as triethylamine or pyridine, alkali metal carbonates, eg. sodium carbonate or potassium carbonate, and alkali metal hydrides, eg. sodium hydride. Triethylamine and pyridine are preferably used.
- 45

110

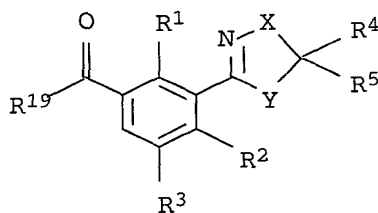
Examples of suitable solvents are chlorinated hydrocarbons such as methylene chloride or 1,2-dichlorethane, aromatic hydrocarbons, eg. toluene, xylene or chlorobenzene, ethers such as diethyl ether, methyl tert-butyl ether, tetrahydrofuran or dioxane, polar aprotic solvents such as acetonitrile, dimethylformamide or dimethyl sulfoxide, or esters such as ethyl acetate, or mixtures of these.

As a rule, the reaction temperature is in the range of from 0°C to the boiling point of the reaction mixture.

Work-up can be effected in a manner known per se to give the product.

Those pyrazoles of the formula II (where Z = H) which are used as starting materials and which are not already known can be prepared by processes known per se (for example EP-A 240 001 and J. Prakt. Chem. 315, 383 (1973)).

Novel 3-heterocyclyl-substituted benzoic acid derivatives of the formula III



III

are those where the variables have the following meanings:

R¹, R² are hydrogen, nitro, halogen, cyano, C₁-C₆-alkyl, C₁-C₆-haloalkyl, C₁-C₆-alkoxy, C₁-C₆-haloalkoxy, C₁-C₆-alkylthio, C₁-C₆-haloalkylthio, C₁-C₆-alkylsulfinyl, C₁-C₆-haloalkylsulfinyl, C₁-C₆-alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;

R³ is hydrogen, halogen or C₁-C₆-alkyl;

R⁴, R⁵ are hydrogen, halogen, cyano, nitro, C₁-C₄-alkyl, C₁-C₄-alkoxy-C₁-C₄-alkyl, di(C₁-C₄-alkoxy)-C₁-C₄-alkyl, di(C₁-C₄-alkyl)amino-C₁-C₄-alkyl, [2,2-di(C₁-C₄-alkyl)hydrazino-1]-C₁-C₄-alkyl, C₁-C₆-alkyliminoxy-C₁-C₄-alkyl,

111

- C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl,
 C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C₁-C₄-alkoxy,
 C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy, hydroxyl,
 C₁-C₄-alkylcarbonyloxy, C₁-C₄-alkylthio,
 C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶, phenyl or
 benzyl, it being possible for the two last-mentioned
 substituents to be partially or fully halogenated and/or
 to have attached to them one to three of the following
 groups:
 nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy
 or C₁-C₄-haloalkoxy;
- or
- R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be
 mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can
 be interrupted by oxygen or by a nitrogen which is
 unsubstituted or substituted by C₁-C₄-alkyl;
- or
- R⁴ and R⁵ together with the corresponding carbon form a carbonyl
 or a thiocarbonyl group;
- R⁶ is hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy,
 C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy,
 C₃-C₆-alkenyloxy, C₃-C₆-alkynyloxy or NR⁷R⁸;
- R⁷ is hydrogen or C₁-C₄-alkyl;
- R⁸ is C₁-C₄-alkyl;
- X is O, S, NR⁹, CO or CR¹⁰R¹¹;
- Y is O, S, NR¹², CO or CR¹³R¹⁴;
- R⁹, R¹² are hydrogen or C₁-C₄-alkyl;
- R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or CONR⁷R⁸;
- or

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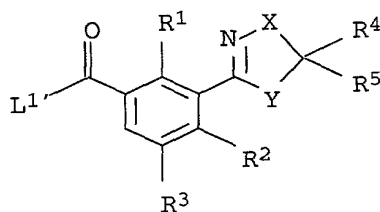
R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

R¹⁹ is hydroxyl or a radical which can be removed by hydrolysis;

with the exception of methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate, methyl 2-chloro-3-(4,5-dihydrooxazol-2-yl)-4-methylsulfonylbenzoate and methyl 2,4-dichloro-3-(5-methylcarbonyloxy-4,5-dihydroisoxazol-3-yl)-benzoate.

Examples of radicals which can be removed by hydrolysis are alkoxy, phenoxy, alkylthio and phenylthio radicals which are unsubstituted or substituted, halides, hetaryl radicals which are bonded via nitrogen; amino, imino radicals which are unsubstituted or substituted, and the like.

Preferred are 3-heterocycl-yl-substituted benzoic acid halides of the formula IIIa', where L^{1'} = halogen (\cong III where R¹⁹ = halogen)



IIIa'

where the variables R¹ to R⁵, X and Y have the meanings given under the formula III and

L^{1'} is halogen, in particular chlorine or bromine.

Equally preferred are 3-heterocycl-yl-substituted benzoic acids of the formula III β (\cong III where R¹⁹ = hydroxyl)

5



Equally preferred are 3-heterocyclyl-substituted benzoic esters
15 of the formula IIIγ (\cong III where R¹⁹ = C₁-C₆-alkoxy)



L^3 is C_1-C_6 -alkoxy.

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40 R^1 is halogen, C_1 - C_6 -alkyl, C_1 - C_6 -alkylthio or
 C_1 - C_6 -alkylsulfonyl;
in particular chlorine, methyl, methylthio or
methylsulfonyl;
extraordinarily preferably chlorine;

45 R² is hydrogen, nitro, halogen, C₁-C₆-alkylthio,
C₁-C₆-alkylsulfinyl or C₁-C₆-alkylsulfonyl;

in particular hydrogen, nitro, chlorine, methylthio, methylsulfinyl, methylsulfonyl, ethylsulfonyl or propylsulfonyl;

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 \mathbb{R}^3

10 R^4, R^5

15

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or

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or

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 \mathbb{R}^6

40 X

Y

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R^{10} , R^{11} , R^{13} , R^{14} are hydrogen, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl or C_1 - C_4 -alkoxycarbonyl;
in particular hydrogen, methyl, chloromethyl or methoxycarbonyl;

5

or

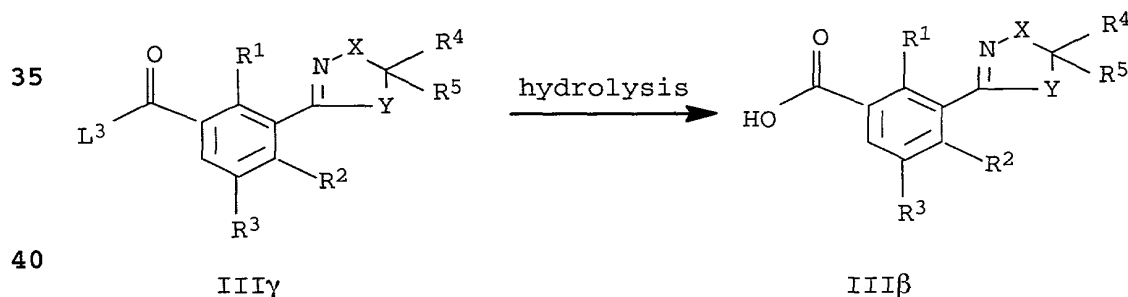
R^5 and R^{13} together form a C_2 - C_6 -alkanediyl chain which can be mono- to polysubstituted by C_1 - C_4 -alkyl and/or which can
be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C_1 - C_4 -alkyl;
in particular 1,3-propanediyl;

R^{19} is hydroxyl, halogen or C_1 - C_6 -alkoxy;
in particular hydroxyl, chlorine, methoxy or ethoxy;

with the exception of methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate, methyl 2-chloro-3-(4,5-dihydroisoxazol-2-yl)-4-methylsulfonylbenzoate and methyl 2,4-dichloro-3-(5-methylcarbonyloxy-4,5-dihydroisoxazol-3-yl)benzoate.

The benzoyl halides of the formula $III\alpha'$ (where $L^1 = Cl, Br$) can be prepared in a manner known per se by reacting the benzoic acids of the formula $III\beta$ with halogenating reagents such as
thionyl chloride, thionyl bromide, phosgene, diphosgene, triphosgene, oxalyl chloride or oxalyl bromide.

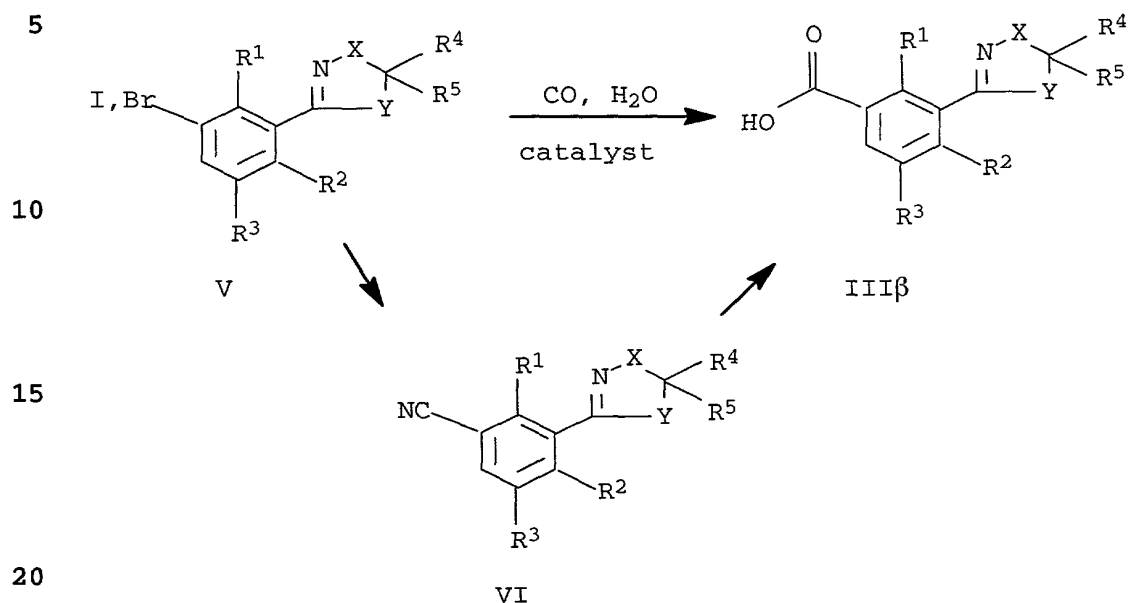
The benzoic acids of the formula $III\beta$ can be prepared in a known manner from the corresponding esters of the formula $III\gamma$ ($L^3 = C_1$ - C_6 -alkoxy) by means of acid or basic hydrolysis.



Equally, the benzoic acids of the formula $III\beta$ can be obtained by reacting corresponding bromine- or iodine-substituted compounds
of the formula V, with carbon monoxide and water under elevated

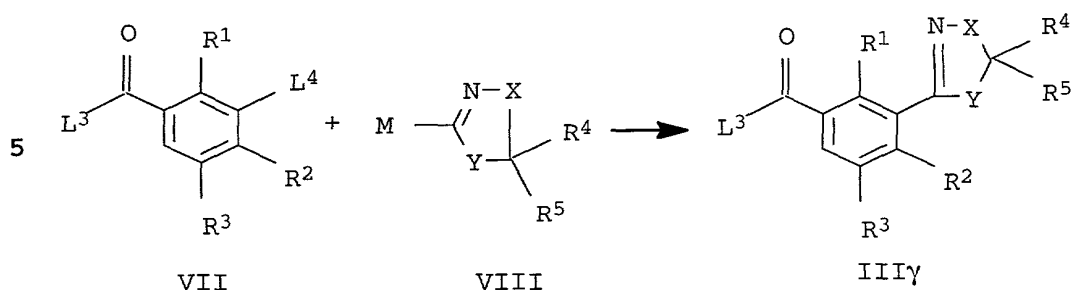
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pressure in the presence of a palladium, nickel, cobalt or rhodium transition metal catalyst and a base.



Furthermore, it is possible to convert compounds of the formula V into the corresponding nitriles of the formula VI by a Rosenmund-von Braun reaction (cf., for example, Org. Synth. Vol III (1955), 212) and to convert these nitriles into the compounds of the formula IIIβ by subsequent hydrolysis.

The esters of the formula IIIγ can be obtained by reacting arylhalogen compounds or arylsulfonates of the formula VII, where L⁴ is a leaving group such as bromine, iodine, triflate, fluorosulfonyloxy and the like with heterocyclyl stannates (Stille couplings), heterocyclyl-boron compounds (Suzuki couplings) or heterocyclyl-zinc compounds (Negishi reaction) VIII, where M is Sn(C₁-C₄-alkyl)₃, B(OH)₂, ZnHal (where Hal = chlorine, bromine) and the like, respectively, in a manner known per se (cf., for example, Tetrahedron Lett. 27 (1986), 5269) in the presence of a palladium or nickel transition metal catalyst and in the presence or absence of a base.

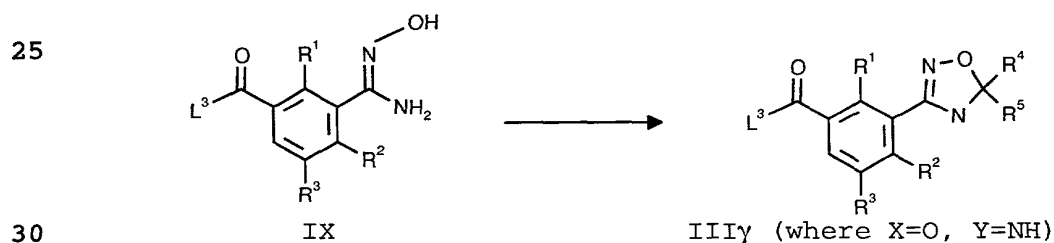


- 10 (where $L^4 = \text{Br, I, OSO}_2\text{CF}_3, \text{OSO}_2\text{F}$) (where $M = \text{Sn}(\text{C}_1\text{-C}_4\text{-Alkyl})_3, \text{B}(\text{OH})_2, \text{ZnHal}$, where Hal is Cl or Br)

15

Equally, it is possible to obtain esters of the formula IIIy by synthesizing the heterocycle which is bonded in the 3-position.

- 20 For example, 1,2,4-oxadiazolin-3-yl derivatives (IIIy where $X=\text{O}$, $Y=\text{NH}$) can be prepared from amidoximes of the formula IX by condensation with aldehydes or ketones (cf., for example, Arch. Phar. 326 (1993), 383-389).



Thioamides of the formula X are suitable precursors for 2-thiazoliny derivatives I (where $X=\text{CR}^{10}\text{R}^{11}$, $Y=\text{S}$) (cf., for example, Tetrahedron 42 (1986), 1449-1460).

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2-Oxazolinyl, 2-thiazolinyl and 2-imidazolinyl derivatives (III_Y where X=CR¹⁰R¹¹, Y=O or Y=S or Y=NH) are accessible from the carboxylic acids of the formula XI (cf., for example, Tetrahedron Let. 22 (1981), 4471-4474).

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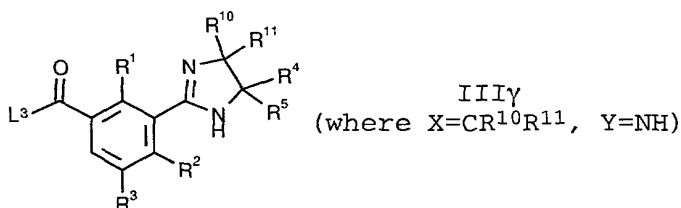
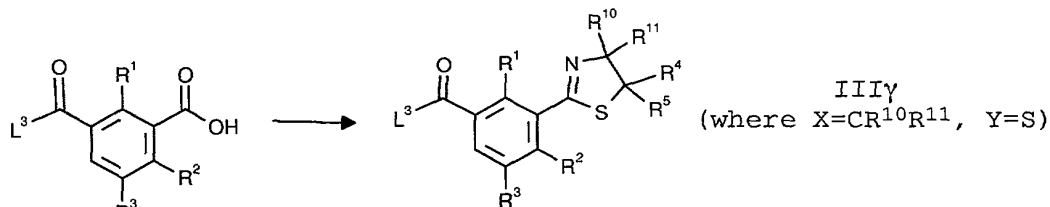
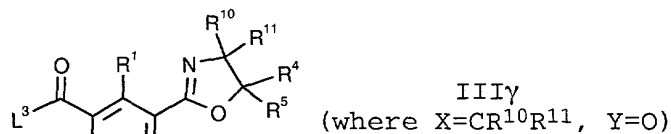
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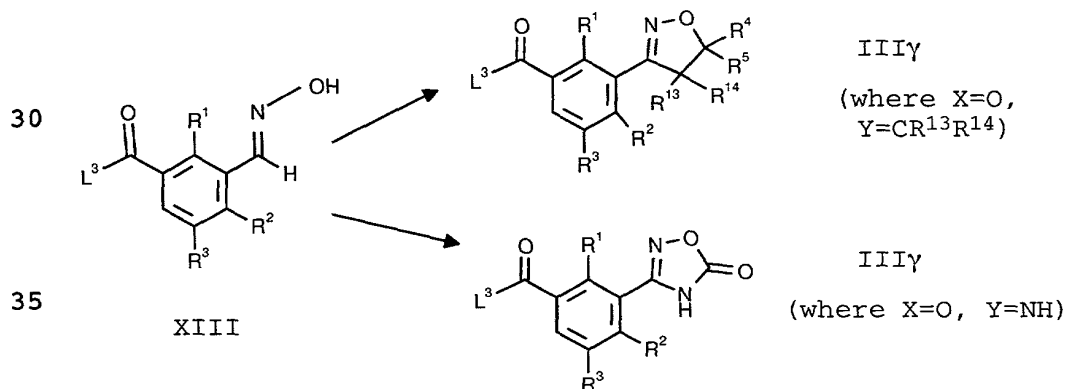
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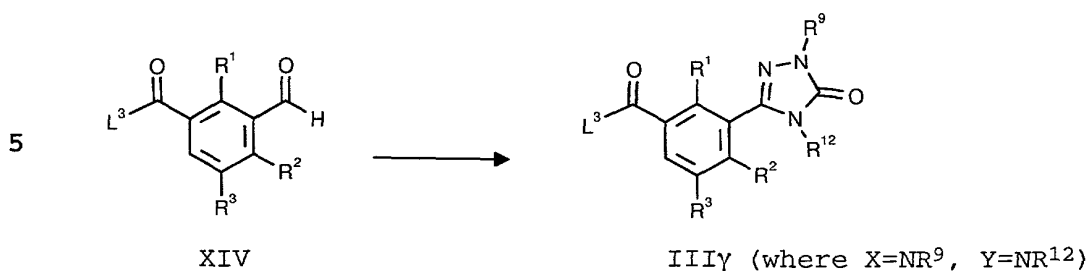


1,3-Thiazol-5(4H)-thion-2-yl (cf., for example, Helv. Chim. Acta 69 (1986), 374-388) and 5-oxo-2-imidazolin-2-yl derivatives (cf., for example, Heterocycles 29 (1989), 1185-1189) (III where X=CR¹⁰R¹¹, Y=S or Y=NH) can be prepared by processes known from the literature from carboxylic acid halides of the formula XII where Hal is halogen, in particular from carboxylic acid chlorides.

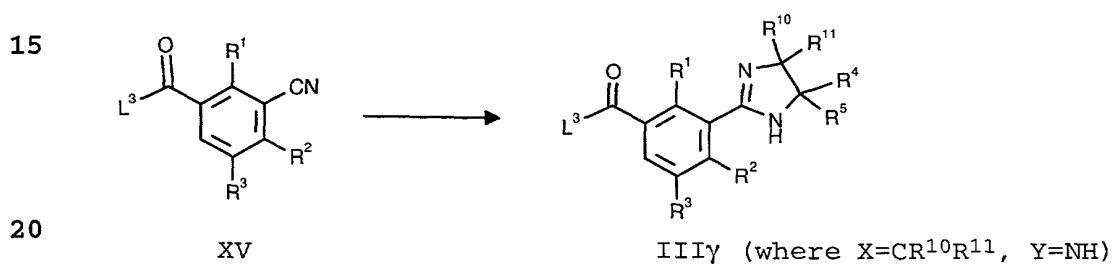
The oximes of the formula XIII can be converted into 4,5-dihydroisoxazol-3-yl derivatives (IIIIy where X=O, Y=CR¹³R¹⁴) in a manner known per se via the hydroxamic acid chlorides XIV as intermediates. From the latter, nitrile oxides are prepared in situ, and these nitrile oxides react with alkenes to give the desired products (cf., for example, Chem. Ber. 106 (1973), 3258-3274). 1,3-Dipolar cycloaddition reactions of chlorosulfonyl isocyanate with nitrile oxides yield 1,2,4-oxadiazolin-5-on-3-yl derivatives (IIIIy where X=O, Y=NH) (cf., for example, Heterocycles 27 (1988), 683-685).



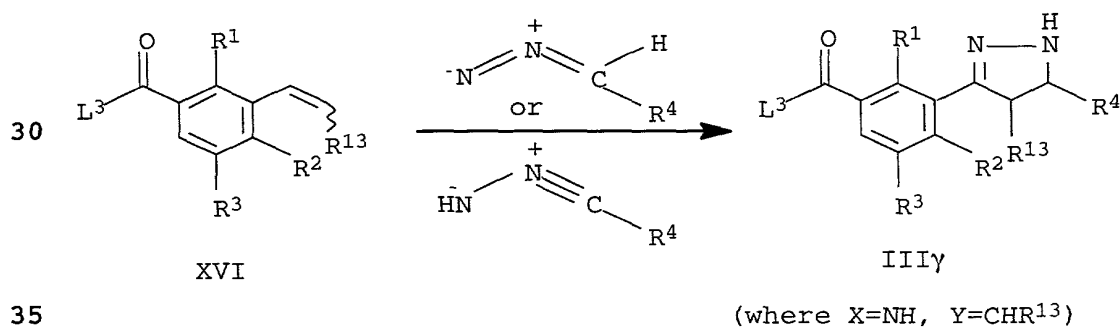
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- 10 2-Imidazoliny derivatives (IIIy where X=CR¹⁰R¹¹, Y=NH) can also be prepared from benzonitriles of the formula XV using known methods (cf., for example, J. Org. Chem. 52 (1987), 1017-1021).



- 1,3-Dipolar cycloaddition reactions of diazoalkanes or nitriloimines with arylalkenes of the formula XVI can be used for synthesizing 3-pyrazoliny derivatives (IIIy where X=NH, Y=CHR¹³).
- 25



- The bromine- or iodine-substituted compounds of the formula V which are used as starting compounds can be obtained from corresponding anilines by methods similar to those known from the literature, for example by Sandmeyer reaction, and the anilines, in turn, are synthesized by reducing suitable nitro compounds. The bromine-substituted compounds of the formula V can additionally be obtained by direct bromination of suitable starting materials (cf. Monatsh. Chem. 99 (1968), 815-822).
- 40
- 45

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The nitriles of the formula VI can be obtained as described above. Equally, it is possible to synthesize them from corresponding anilines by means of a Sandmeyer reaction.

- 5 The starting compounds of the formula VII are known (cf., for example, Coll. Czech. Chem. Commun. 40 (1975), 3009-3019) or can be prepared readily by a suitable combination of known syntheses.
- 10 For example, the sulfonates VII ($L^4 = \text{OSO}_2\text{CF}_3, \text{OSO}_2\text{F}$) can be obtained from the corresponding phenols, which, in turn, are known (cf., for example, EP-A 195 247) or can be prepared by known methods (cf., for example, Synthesis 1993, 735-762).
- 15 The halogen compounds VII ($L^4 = \text{Cl}, \text{Br}$ or I) can be obtained, for example, from the corresponding anilines of the formula XIX by a Sandmeyer reaction.

- The amidoximes of the formula IX, the thioamides of the formula X
- 20 and the carboxylic acids of the formula XI can be synthesized from the nitriles of the formula XV in a manner known per se.

- Furthermore, it is possible to prepare the carboxylic acids of the formula XI from the aldehydes of the formula XIV by known
- 25 processes (cf., for example, J. March, Advanced Organic Chemistry, 3rd edition (1985), p. 629 et seq., Wiley-Interscience Publication).

- 30 The carboxylic acid halides of the formula XII can be obtained from the corresponding carboxylic acids of the formula XI by methods similar to standard processes.

- The oximes of the formula XIII are advantageously obtained by
- 35 reacting aldehydes of the formula XIV with hydroxylamine in a manner known per se (cf., for example, J. March, Advanced Organic Chemistry, 3rd ed. (1985), pp. 805-806, Wiley-Interscience Publication).

- 40 Those aldehydes of the formula XIV which are not already known can be prepared by methods similar to known processes. Thus, they can be synthesized from methyl compounds of the formula XVII by means of bromination, for example with N-bromosuccinimide or 1,3-dibromo-5,5-dimethylhydantoin, followed by oxidation (cf.
- 45 Synth. Commun. 22 (1992), 1967 - 1971).

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The oximes of the formula XIII can also be converted into nitriles of the formula XV by processes which are known per se (cf., for example, J. March, Advanced Organic Chemistry, 3rd ed. (1985), pp. 931-932, Wiley-Interscience Publication).

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Arylalkenes of the formula XVI can be synthesized starting from the halogen compounds or sulfonates of the formula VII ($L^4 = \text{Br}, \text{Cl}, \text{OSO}_2\text{CF}_3, \text{OSO}_2\text{F}$) by, inter alia, Heck reaction with olefins in the presence of a palladium catalyst (cf., for example, Heck,

10 Palladium Reagents in Organic Synthesis, Academic Press, London 1985; Synthesis 1993, 735 - 762).

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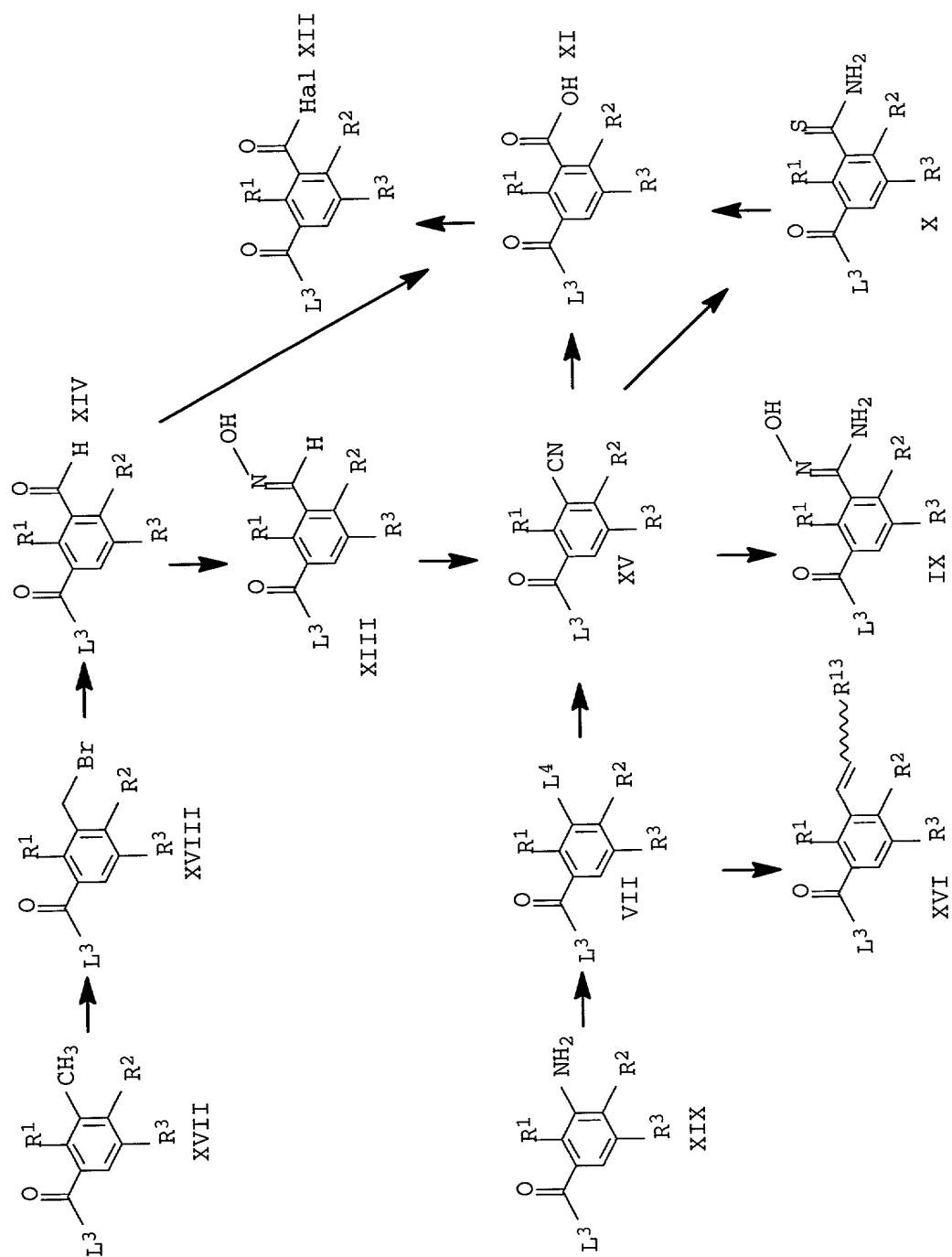
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Preparation examples:

- 5 4-[2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-5-hydroxy-1-methyl-1H-pyrazole (compound 3.35)

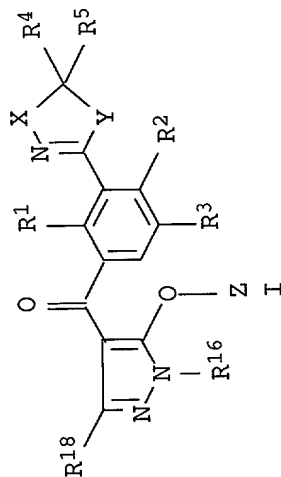
- 10 43.60 g (0.13 mol) of 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride in 375 ml of anhydrous dioxane and 13.56 g (0.134 mol) of triethylamine in 375 ml of anhydrous dioxane are simultaneously added dropwise at room temperature under a protective gas atmosphere to a solution 12.74 g (0.13 mol) of 5-hydroxy-1-methylpyrazole and 300 ml of anhydrous dioxane. After the reaction mixture had been stirred 15 for 2 hours at room temperature, it was filtered through silica gel and the residue was washed with dioxane. The eluate was concentrated in vacuo to approximately 500 ml, and 17.94 g (0.13 mol) of dried, finely powdered potassium carbonate were added. After the mixture had been refluxed for 6 hours, the 20 solvent was distilled off in vacuo and the residue was taken up in approximately 700 ml of water. Insoluble constituents were filtered off, and the pH of the filtrate was brought to 2 - 3 by slow addition of 10% strength hydrochloric acid. The precipitate which formed was filtered off with suction. This gave 46.16 g 25 (92% of theory) of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-5-hydroxy-1-methyl-1H-pyrazole. (m.p. > 250°C)

- 30 Table 3 shows the above compound and, in addition, other 3-heterocyclyl-substituted benzoyl derivatives of the formula I which were prepared, or can be prepared, in a similar manner (if the end products had not precipitated upon acidification with 10% strength hydrochloric acid, they were extracted with ethyl acetate or dichloromethane; the organic phase was subsequently 35 dried and concentrated in vacuo):

40

45

Table 3:



No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.1	Cl	Cl	H	O	H	H	CH ₂	n-C ₄ H ₉	H	H	116 - 117
3.2	Cl	Cl	H	O	H	H	CH ₂	i-C ₄ H ₉	H	H	148 - 151
3.3	Cl	Cl	H	O	H	H	CH ₂	n-C ₄ H ₉	C ₂ H ₅ SO ₂	H	0.95 (t); 1.32 (m); 1.62 (t); 1.92 (quin); 3.30 (t); 3.78 (quar); 4.17 (t); 4.61 (t); 7.42 (d); 7.48 (m).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.4	Cl	Cl	H	O	H	H	CH ₂	i-C ₄ H ₉	i-C ₄ H ₉ SO ₂	H	0.96 (d); 1.21 (d); 2.33 (m); 2.48 (m); 3.30 (t); 3.67 (d); 3.97 (d); 4.58 (t); 7.42 (d); 7.50 (m).
3.5	Cl	Cl	H	O	H	H	CH ₂	n-C ₃ H ₇	i-C ₄ H ₉ SO ₂	H	0.97 (t); 1.20 (d); 1.96 (m); 2.49 (m); 3.30 (t); 3.68 (d); 4.12 (t); 4.59 (t); 7.42 (d); 7.49 (d); 7.52 (s).
3.6	Cl	Cl	H	O	H	H	CH ₂	n-C ₃ H ₇	C ₂ H ₅ SO ₂	H	0.97 (t); 1.12 (d); 1.63 (t); 1.94 (m); 3.29 (t); 3.76 (q); 4.14 (t); 4.60 (t); 7.42 (d); 7.48 (d); 7.51 (s).
3.7	Cl	SO ₂ CH ₃	H	O	COOC ₂ H ₅	H	CH ₂	CH ₃	H	H	70 - 75
3.8	Cl	SO ₂ CH ₃	H	O	COOC ₂ H ₅	H	CH ₂	C ₂ H ₅	H	H	65 - 70
3.9	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	CH ₃	H	H	230 - 235
3.10	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	C ₂ H ₅	H	H	210 - 215
3.11	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	n-C ₃ H ₇	H	H	95 - 100
3.12	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	CH ₃	C ₂ H ₅ SO ₂	H	70 - 75

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.13	C1	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	C ₂ H ₅	C ₂ H ₅ SO ₂	H	78 - 83
3.14	C1	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	C ₂ H ₅	i-C ₄ H ₉ SO ₂	H	1.24 (2d); 1.53 (t); 2.52 (m); 3.05 (dd); 3.29 (s); 3.52 (dd); 3.73 (d); 4.24 (q), 5.05 (m); 7.49 (s); 7.66 (d); 8.18 (d).
3.15	C1	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	n-C ₃ H ₇	C ₂ H ₅ SO ₂	H	0.96 (t); 1.53 (d); 1.68 (t); 1.95 (sext); 3.07 (dd); 3.32 (s); 3.58 (dd); 3.86 (quart); 4.15 (t); 5.03 (m); 7.46 (d); 7.64 (d); 8.18 (d).
3.16	C1	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	CH ₃	H	H	220 - 225
3.17	C1	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	C ₂ H ₅	H	H	82 - 86
3.18	C1	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	n-C ₃ H ₇	H	H	70 - 75
3.19	C1	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	n-C ₄ H ₉	H	H	68 - 73
3.20	C1	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	i-C ₄ H ₉	H	H	45 - 50
3.21	C1	SO ₂ CH ₃	H	O	C ₂ H ₅	H	CH ₂	CH ₃	H	H	220 - 225
3.22	C1	SO ₂ CH ₃	H	O	C ₂ H ₅	H	CH ₂	C ₂ H ₅	H	H	170 - 175

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.23	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	n-C ₃ H ₇	H	H	65 - 70
3.24	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	n-C ₄ H ₉	H	H	55 - 60
3.25	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	i-C ₄ H ₉	H	H	58 - 63
3.26	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	n-C ₄ H ₉	C ₂ H ₅ SO ₂	H	78 - 83
3.27	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	n-C ₄ H ₉	i-C ₄ H ₉ SO ₂	H	0.94 (t); 1.19 (d); 1.22 (t); 1.38 (m); 1.74 (br); 1.91 (m); 2.53 (m); 3.26 (s); 4.45 (t); 3.76 (d); 4.18 (t); 4.62 (t); 7.45 (s); 7.64 (d); 8.16 (d).
3.28	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	i-C ₄ H ₉	i-C ₄ H ₉ SO ₂	H	0.96 (d); 1.21 (d); 2.33 (m); 2.51 (m); 3.28 (s); 3.44 (t); 3.75 (d); 3.99 (d); 4.61 (t); 7.45 (s); 7.66 (d); 8.17 (d).
3.29	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	i-C ₄ H ₉	C ₂ H ₅ SO ₂	H	0.97 (d); 1.66 (t); 2.36 (m); 3.29 (s); 3.43 (t); 3.82 (q); 3.99 (d); 4.60 (t); 7.47 (s); 7.68 (d); 8.18 (d).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.30	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	C ₂ H ₅ SO ₂	H	1.68(t); 3.29(s); 3.43(t); 3.78(q); 3.92(s); 3.63(t); 7.46(s); 7.62(d); 8.17(d).
3.31	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	i-C ₄ H ₉ SO ₂	H	1.23(d); 2.53(m), 3.28(s); 3.43(t); 3.70(d); 3.91(s); 4.61(t); 7.48(s); 7.66(d); 8.18(d).
3.32	Cl	Cl	H	O	H	H	CH ₂	n-C ₃ H ₇	H	H	119 - 121
3.33	Cl	Cl	H	O	H	H	CH ₂	CH ₃	H	CH ₃	115 - 117
3.34	Cl	NO ₂	H	O	H	H	CH ₂	C ₂ H ₅	H	H	217 - 218
3.35	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	H	H	> 250
3.36	Cl	Cl	H	O	H	H	CH ₂	C ₂ H ₅	H	H	125 - 128
3.37	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	n-C ₃ H ₇ SO ₂	H	78 - 83
3.38	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	C ₂ H ₅ SO ₂	H	1.52(t); 1.68(t); 3.29(s); 3.43(t); 3.82(q); 4.24(q); 4.63(t); 7.48(s); 7.65(d); 8.07(d).
3.39	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	CH ₃	CH ₂	CH ₃	H	H	> 200
3.40	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	H	CH ₂	CH ₃	H	H	220 - 223

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.41	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	H	CH ₂	C ₂ H ₅	H	H	> 230
3.42	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	H	CH ₂	CH ₃	H	H	1.12(t); 1.53(d); 1.76(quin); 3.18(dd); 3.38(t); 3.55(dd); 3.73(s); 5.04(m); 5.55(s,br.); 7.37(s); 7.68(d); 8.13(d).
3.43	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	H	CH ₂	C ₂ H ₅	H	H	1.07(t); 1.50(m); 1.78(quin); 3.07(dd); 3.39(t); 3.55(dd); 4.12(t); 5.08(m); 7.38(s); 7.69(d); 8.11(d).
3.44	Cl	SO ₂ CH ₃	H	CH ₂	H	H	O	CH ₃	H	H	
3.45 a)	Cl	SO ₂ CH ₃	H	C(CH ₃) ₂	H	H	O	CH ₃	H	H	1.33(s); 3.40(s); 4.17(s); 7.43(s); 7.79(d); 8.04(d).
3.46	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	Na ⁺	H	218 - 220
3.47	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	K ⁺	H	193
3.48	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	Li ⁺	H	> 230
3.49	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	NH ₄ ⁺	H	170 - 175

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
3.50	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	Na ⁺	H	> 240
3.51	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	K ⁺	H	206 - 214
3.52	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	Li ⁺	H	> 240
3.53	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	NH ₄ ⁺	H	
3.54 a)	Cl	SO ₂ CH ₃	H	C(CH ₃) ₂	H	H	O	C ₂ H ₅	H	H	1.27(t); 1.36(s); 3.41(q); 4.01(q); 4.18(s); 7.47(s); 7.83(d); 8.07(d).
3.55	Cl	SO ₂ CH ₃	H	O	H	-(CH ₂) ₃ CH-		C ₂ H ₅	H	H	99-104
3.56	Cl	SO ₂ CH ₃	H	O	H	-(CH ₂) ₃ CH-		CH ₃	H	H	95-100
3.57	Cl	SO ₂ CH ₃	H	O		-(CH ₂) ₄ -	CH ₂	CH ₃	H	H	230-235
3.58	Cl	SO ₂ CH ₃	H	O		-(CH ₂) ₄ -	CH ₂	C ₂ H ₅	H	H	190-195
3.59	Cl	SO ₂ CH ₃	H	O		-(CH ₂) ₂ O(CH ₂) ₂	CH ₂	C ₂ H ₅	H	H	95-100
3.60	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	CH ₃	CH ₂	CH ₃	H	H	< 230
3.61	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	CH ₃	CH ₂	C ₂ H ₅	H	H	198-200
3.62	Cl	SO ₂ C ₂ H ₅	H	O	H	H	CH ₂	CH ₃	H	H	215-218
3.63	Cl	SO ₂ C ₂ H ₅	H	O	H	H	CH ₂	C ₂ H ₅	H	H	213-215
3.64	Cl	SO ₂ -n-C ₃ H ₇	H	O	H	H	CH ₂	CH ₃	H	H	186-190

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No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; 1H-NMR [δ in ppm]
3.65	Cl	SO ₂ -n-C ₃ H ₇	H	O	H	H	CH ₂	C ₂ H ₅	H	H	84-86
3.66	Cl	SO ₂ CH ₃	H	O	-(CH ₂) ₂ O(CH ₂) ₂ -		CH ₂	CH ₃	H	H	90-95
3.67	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	C ₂ H ₅	CH ₂	CH ₃	H	H	70-75
3.68	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	C ₂ H ₅	CH ₂	C ₂ H ₅	H	H	50-55
3.69	Cl	SO ₂ CH ₃	H	O	OCH ₃	H	CH ₂	CH ₃	H	H	3.18-3.99 (1H); 5.78 (1H); 7.50 (1H); 7.81 (1H); 8.09 (1H).
3.70	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₂ Cl	CH ₃	H	H	1.52 (3H); 3.30-4.12 (8H); 4.36 (1H); 4.93 (1H); 7.49 (1H); 7.81 (1H); 8.09 (1H).
3.71	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₂ Cl	C ₂ H ₅	H	H	1.27 (3H); 1.55 (3H); 3.28-4.02 (7H); 4.37 (1H); 4.92 (1H); 7.48 (1H); 7.80 (1H); 8.07 (1H).
3.72	Cl	SO ₂ CH ₃	H	C(CH ₃) ₂	H	H	O	CH ₃	H	H	132-135
3.73	Cl	SO ₂ CH ₃	H	O	OC ₂ H ₅	H	CH ₂	CH ₃	H	H	95-100
3.74	Cl	SO ₂ CH ₃	H	O	OC ₂ H ₅	H	CH ₂	C ₂ H ₅	H	H	1.16 (3H); 1.27 (3H); 3.20-4.00 (9H); 5.89 (1H); 7.50 (1H); 7.82 (1H); 8.07 (1H).
3.75	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	C ₂ H ₅	CH ₂	C ₂ H ₅	K ⁺	H	200-205

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; 1H-NMR [δ in ppm]
3.76	Cl	SO ₂ C ₂ H ₅	H	C(CH ₃) ₂	H	H	O	CH ₃	H	H	120-123
3.77	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	CH ₃	CH ₂	C ₂ H ₅	H	H	152-158
3.78	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	CH ₃	CH ₂	CH ₃	H	H	172-176
3.79	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	H	CH ₂	CH ₃	H	H	188-205
3.80	Cl	SCH ₃	H	O	H	H	CH ₂	C ₂ H ₅	H	H	1.29(t); 2.56(s); 3.28(t); 3.93(q); 4.49(t); 7.40(s); 7.43(d); 7.55(d).
3.81	Cl	SO ₂ CH ₃	H	O	CH ₂ Cl	H	CH ₂	C ₂ H ₅	H	H	78-82
3.82	CH ₃	H	H	CH ₂	H	H	S	C ₂ H ₅	H	H	1.44(t); 2.50(s); 3.49(t); 4.09(q); 4.53(t); 7.35(m); 7.48(d); 7.62(d).
3.83	Cl	SO ₂ CH ₃	H	O	CH ₂ Cl	H	CH ₂	CH ₃	H	H	81-85
3.84	Cl	SCH ₃	H	O	H	H	CH ₂	CH ₃	H	H	151-153
3.85	Cl	SOCH ₃	H	O	H	H	CH ₂	C ₂ H ₅	H	H	1.28(t); 2.82(s); 3.40(m); 3.92(m); 4.52(t); 7.45(s); 7.82(d); 8.10(d).
3.86	CH ₃	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	H	H	205-210
3.87	Cl	Cl	H	CH ₂	H	H	S	C ₂ H ₅	H	H	173-179
3.88	Cl	SCH ₃	H	CH ₂	H	H	S	C ₂ H ₅	H	H	1.43(t); 2.51(s); 3.59(t); 4.08(q); 4.51(t); 7.22(d); 7.41(s); 7.50(d).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; ¹ H-NMR [δ in ppm]
3.89	Cl	SO ₂ CH ₃	H	CH ₂	H	H	S	C ₂ H ₅	H	H	1.50(t); 3.28(s); 3.62(t); 4.10(q); 4.49(t); 7.36(s); 7.68(d); 8.19(d).
3.90	CH ₃	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	H	H	174-180
3.91	Cl	SO ₂ CH ₃	H	O	CH ₂ Cl	H	CH ₂	CH ₃	H	H	77-83
3.92	Cl	SO ₂ CH ₃	H	O	F	H	CH ₂	CH ₃	H	H	
3.93	Cl	SO ₂ CH ₃	H	O	F	H	CH ₂	C ₂ H ₅	H	H	
3.94	Cl	SO ₂ CH ₃	H	O	F	F	CH ₂	CH ₃	H	H	
3.95	Cl	SO ₂ CH ₃	H	O	F	F	CH ₂	C ₂ H ₅	H	H	
3.96	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	C ₂ H ₅	H	H	183-184
3.97	Cl	SO ₂ CH ₃	H	O	CF ₃	H	CH ₂	CH ₃	H	H	223-225
3.98	Cl	SO ₂ CH ₃	H	O	CF ₃	H	CH ₂	C ₂ H ₅	H	H	183-184
3.99	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	CH ₃	H	H	195-196
3.100	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	C ₂ H ₅	H	H	199-200
3.101	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	CH ₃	H	H	230-233
3.102	Cl	SO ₂ CH ₃	H	O	CHCl(CH ₃)	H	CH ₂	C ₂ H ₅	H	H	102-107
3.103	Cl	SO ₂ CH ₃	H	O	CHCl(CH ₃)	H	CH ₂	CH ₃	H	H	80-85
3.104	Cl	SO ₂ CH ₃	H	O	n-C ₃ H ₇	H	CH ₂	CH ₃	H	H	
3.105	Cl	SO ₂ CH ₃	H	O	n-C ₃ H ₇	H	CH ₂	C ₂ H ₅	H	H	
3.106	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	⁺ NH ₂ (CH ₃) ₂	H	200

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁶	Z	R ¹⁸	Physical data m.p. [°C]; 1H-NMR [δ in ppm]
3.107	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	+NH ₂ (CH ₂ CH ₂ OH)	H	187
3.108	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	+NH ₃ (CH ₂ CH ₂ OCH ₂ CH ₂ OH)	H	180
3.109	SCH ₃	SCH ₃	H	O	H	H	CH ₂	CH ₃	H	H	2.33(s); 2.51(s); 3.40(t); 3.70(s); 4.58(t); 5.15(brs); 7.21(s); 7.31(d); 7.42(d).
3.110	SCH ₃	SCH ₃	H	O	H	H	CH ₂	C ₂ H ₅	H	H	1.38(t); 2.33(s); 2.49(s); 3.41(t); 4.10(q); 4.58(t); 7.25(s); 7.32(d); 7.41(d); 7.82(brs).
3.111	SO ₂ CH ₃	SO ₂ CH ₃	H	O	H	H	CH ₂	CH ₃	H	H	oil
3.112	SO ₂ CH ₃	SO ₂ CH ₃	H	O	H	H	CH ₂	C ₂ H ₅	H	H	oil

a) Prepared from 2-chloro-3-(1'-chloro-2',2'-dimethylethylaminocarbonyl)-4-methylsulfonylbenzoyl chloride with two equivalents of potassium carbonate.

The syntheses of some starting materials are given below:

- 5 2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride (compound 4.5)

Step a) 2-Chloro-3-methyl-4-methylthioacetophenone

- 10 A solution of 157 g (2 mol) of acetyl chloride in 420 ml of 1,2-dichloroethane was added dropwise to a suspension of 286 g (2.14 mol) of aluminum trichloride in 420 ml of 1,2-dichloroethane at 15-20°C. A solution of 346 g (2 mol) of 2-chloro-6-methylthiotoluene in 1 l of 15 1,2-dichloroethane was subsequently added dropwise. After the reaction mixture had been stirred for 12 hours, it was poured into a mixture of 3 l of ice and 1 l of concentrated HCl. The mixture was extracted with methylene chloride, and the organic phase was washed with 20 water, dried with sodium sulfate and concentrated. The residue was distilled in vacuo. This gave 256 g (60% of theory) of 2-chloro-3-methyl-4-methylthioacetophenone. (m.p.: 46°C)

- 25 Step b) 2-Chloro-3-methyl-4-methylsulfonylacetophenone

- 163.0 g (0.76 mol) of 2-chloro-3-methyl-4-methylthioacetophenone were dissolved in 1.5 l of glacial acetic acid, 18.6 g of sodium tungstate were added, and 30 173.3 g of a 30% strength hydrogen peroxide solution were added dropwise with cooling. Stirring was continued for 2 days and the mixture was subsequently diluted with water. The solid which had precipitated was filtered off with suction, washed with water and dried. This gave 164.0 g 35 (88% of theory) of 2-chloro-3-methyl-4-methylsulfonylacetophenone. (m.p.: 110-111°C)

- 40 Step c) 2-Chloro-3-methyl-4-methylsulfonylbenzoic acid

- 82 g (0.33 mol) of 2-chloro-3-methyl-4-methylsulfonylacetophenone were dissolved in 700 ml of dioxane, and 1 l of a 12.5% strength sodium hypochlorite solution 45 was added at room temperature. Stirring was continued for 1 hour at 80°C. After cooling, two phases formed, of which the bottom phase was diluted with water and

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acidified weakly. The solid which had precipitated was filtered off with suction, washed with water and dried. This gave 60 g (73% of theory) of 2-chloro-3-methyl-4-methylsulfonylbenzoic acid.

5 (m.p.: 230-231°C)

Step d) Methyl 2-chloro-3-methyl-4-methylsulfonylbenzoate

10 100 g (0.4 mol) of 2-chloro-3-methyl-4-methyl-sulfonylbenzoic acid were dissolved in 1 l of methanol and hydrogen chloride gas was passed in for 5 hours at reflux temperature. The mixture was subsequently concentrated. This gave 88.5 g (84% of theory) of methyl 2-chloro-3-methyl-4-methylsulfonylbenzoate.

15 (m.p.: 107-108°C)

Step e) Methyl 3-bromomethyl-2-chloro-4-methylsulfonylbenzoate

20 82 g (0.1 mol) of methyl 2-chloro-3-methyl-4-methyl-sulfonylbenzoate are dissolved in 2 l of tetrachloromethane, and 56 g (0.31 mol) of N-bromosuccinimide are added in portions with exposure to light. The reaction mixture was filtered, the filtrate

25 was concentrated, and the residue was taken up in 200 ml of methyl tert-butyl ether. The solution was treated with petroleum ether and the solid which had precipitated was filtered off with suction and dried. This gave 74.5 g (70% of theory) of methyl 3-bromomethyl-2-chloro-4-methylsulfonylbenzoate.

30 (m.p.: 74-75°C)

Step f) Methyl 2-chloro-3-formyl-4-methylsulfonylbenzoate

35 A solution of 41.0 g (0.12 mol) of methyl 3-bromomethyl-2-chloro-4-methylsulfonylbenzoate in 250 ml of acetonitrile was treated with 42.1 g (0.36 mol) of N-methylmorpholine N-oxide. The batch was stirred for 12 hours at room temperature and subsequently

40 concentrated, and the residue was taken up in ethyl acetate. The solution was extracted with water, dried with sodium sulfate and concentrated. This gave 31.2 g (94% of theory) of methyl 2-chloro-3-formyl-4-methylsulfonylbenzoate

45 (m.p.: 98-105°C)

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Step g) 2-Chloro-3-hydroxyiminomethyl-4-methylsulfonylbenzoic acid

5 15.00 g (54 mmol) of methyl 2-chloro-3-formyl-4-methylsulfonylbenzoate and 4.20 g (60 mmol) of hydroxylamine hydrochloride were taken up in 300 ml of methanol, and a solution of 3.18 g (30 mmol) of sodium carbonate in 80 ml of water was added dropwise. After the mixture had been stirred for 12 hours at room temperature, the methanol was distilled off, the residue was diluted with water and the mixture was extracted with diethyl ether. After the organic phase had been dried, the solvent was removed. This gave 14.40 g (91% of theory) of methyl 2-chloro-3-hydroxyiminomethyl-4-methylsulfonylbenzoate. 15 (m.p.: 126-128°C).

Step h) Methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate (compound 4.3)

20 Ethylene was passed for 30 minutes at 15-20°C into a solution of 158.0 g (0.54 mol) of methyl 2-chloro-3-hydroxyiminomethyl-4-methylsulfonylbenzoate and 1 l of dichloromethane. After 1.6 g of sodium acetate had been added, 454 ml of sodium hypochlorite solution were added dropwise at 10°C while simultaneously passing in ethylene. Ethylene was subsequently passed in at 10°C for a further 15 minutes. After the mixture had been stirred for 12 hours, the phases were separated, and the organic phase was washed with water, dried and concentrated. This gave 156.5 g (90% of theory) of methyl 2-chloro-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate. 25 (1H NMR (δ in ppm): 3.24 (s); 3.42 (t); 3.99 (s); 4.60 (t); 7.96 (d); 8.10 (d)). 35

Step i) 2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid (compound 4.4)

40 A solution of 32.8 g of sodium hydroxide, dissolved in 330 ml of methanol, was slowly added dropwise to a mixture of 170.0 g (0.54 mol) of methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate and 1 l of methanol at 40-45°C. The suspension was stirred for 45 5 hours at 50°C. After the solvent had been distilled off, the residue was taken up in 1.5 l of water, and the aqueous phase was extracted three times with ethyl

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acetate. The aqueous phase was acidified with hydrochloric acid and extracted three times with ethyl acetate. The combined organic phases were subsequently washed to neutrality with water, dried and concentrated.

5 This gave 148.8 g (91% of theory) of 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid.

(¹H NMR (δ in ppm): 3.26 (s); 3.45 (t); 4.63 (t); 8.15 (s); 8.53 (s, br)).

10

Step j) 2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride (compound 4.5)

15

74.8 g (0.63 mol) of thionyl chloride in 50 ml of dry toluene were added dropwise at 50°C to a solution of 139.0 g of 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid, 1 ml of dimethylformamide and 1 l of dry toluene. After the mixture had been heated for 6 hours at 110°C, the solvent was distilled off. This

20

gave 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride in quantitative yield. (¹H NMR (δ in ppm): 3.25 (s); 3.46 (t); 4.62 (t); 8.21 (dd)).

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2-Chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride (compound 4.39)

30

Step a) Methyl 2-chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate (compound 4.25)

35

Propene was passed for 30 minutes at room temperature into a solution of 15.0 g (52 mmol) of methyl 2-chloro-3-hydroxyiminomethyl-4-methylsulfonylbenzoate and 200 ml of dichloromethane. After 1.6 g of sodium acetate had been added, 42.8 ml of sodium hypochlorite solution were added dropwise at room temperature while simultaneously passing in propene. Propene was subsequently passed in for a further 15 minutes at room temperature. After the mixture had been refluxed for 3 hours, it was stirred for 12 hours at room temperature, propene was again passed in for 5 hours under reflux, and the mixture was stirred for a further 12 hours at room temperature. After the phases had been separated, the organic phase was washed with water, dried and concentrated. This gave 15.5 g (89% of theory) of methyl 2-chloro-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methyl-

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sulfonylbenzoate.
(m.p.: 130-135°C).

- 5 Step b) 2-Chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoic acid (compound 4.26)

10 A solution of 3.52 g (88 mmol) of sodium hydroxide, dissolved in 100 ml of methanol, was slowly added dropwise to a mixture of 15.00 g (45 mmol) of methyl 2-chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoate and 200 ml of methanol. The suspension was stirred for 48 hours at room temperature. After the solvent had been distilled off, the residue was taken up in water, and the aqueous phase was washed three times with ethyl acetate. The aqueous phase was acidified with hydrochloric acid and extracted three times with ethyl acetate. The combined organic phases were subsequently washed to neutrality with water, dried and concentrated. This gave 13.20 g (92% of theory) of 2-chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid. (m.p.: 173-178°C).

- 25 Step c) 2-Chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoyl chloride (compound 4.39)

30 5.7 g (51 mmol) of thionyl chloride were added dropwise at room temperature to a solution of 13.0 g (41 mmol) of 2-chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methyl-sulfonylbenzoic acid, 1 ml of dimethylformamide and 250 ml of dry toluene. The mixture was subsequently refluxed until the reaction was complete. After cooling, the solvent was distilled off. This gave 14.2 g of 2-chloro-3-(5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylbenzoyl chloride in quantitative yield.

40 2-Chloro-3-(1'-chloro-2',2'-dimethylethylaminocarbonyl)-4-methyl-sulfonylbenzoyl chloride

- Step a) Methyl 2-chloro-3-hydroxycarbonyl-4-methyl-sulfonylbenzoate

45 13.8 g (0.11 mol) of sodium hydrogen phosphate monohydrate in 170 ml of water, 49.3 g (0.43 mol) of 30% strength hydrogen peroxide solution and 66.2 g (0.59 mol)

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of 80% strength aqueous sodium chlorite solution were added in succession at 5°C to a solution of 115.3 g (0.42 mol) of methyl 2-chloro-3-formyl-4-methylsulfonylbenzoate in 2000 ml of acetonitrile. The reaction solution was subsequently stirred for 1 hour at 5°C and for 12 hours at room temperature. The pH was then brought to 1 with 10% strength hydrochloric acid, and 1500 ml of aqueous 40% strength sodium hydrogen sulfite solution were added. After the mixture had been stirred for 1 hour at room temperature, the aqueous phase was extracted three times with ethyl acetate. The combined organic phases were washed with sodium hydrogen sulfite solution and dried. After the solvent had been distilled off, 102.0 g of methyl 2-chloro-3-hydroxycarbonyl-4-methylsulfonylbenzoate were obtained. (¹H NMR (δ in ppm): 3.34 (s); 3.93 (s); 8.08 (s); 14.50 (s, br.).)

Step b) Methyl 2-chloro-3-chlorocarbonyl-4-methylsulfonylbenzoate

2 drops of dimethylformamide and 11.9 g (0.1 mol) of thionyl chloride were added to a solution of 6.0 g (0.021 mol) of methyl 2-chloro-3-hydroxycarbonyl-4-methylsulfonylbenzoate and 50 ml of dry toluene. The solution was refluxed for 4 hours. After the solvent had been removed in vacuo, 6.2 g of methyl 2-chloro-3-chlorocarbonyl-4-methylsulfonylbenzoate were obtained. (¹H NMR (δ in ppm): 3.21 (s); 4.02 (s); 8.02 (d); 8.07 (d).)

Step c) Methyl 2-chloro-3-(1'-hydroxy-2',2'-dimethylethylaminocarbonyl)-4-methylsulfonylbenzoate

A solution of 7.80 g (25 mmol) of methyl 2-chloro-3-chlorocarbonyl-4-methylsulfonylbenzoate was added dropwise at 0-5°C to a solution of 4.54 g (50 mmol) of 2,2-dimethylethanolamine in 40 ml of dichloromethane. After the reaction solution had been stirred for 6 hours at room temperature, it was extracted three times with water, dried and concentrated. This gave 8.20 g (80% of theory) of methyl 2-chloro-3-(1'-hydroxy-2',2'-dimethylethylaminocarbonyl)-4-methylsulfonylbenzoate. (m.p.: 70-72°C).

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Step d) Methyl 2-chloro-3-(1'-chloro-2',2'-dimethylethylaminocarbonyl)-4-methylsulfonylbenzoate

5 A mixture of 6.9 g (20 mmol) of methyl
2-chloro-3-(1'-hydroxy-2',2'-dimethylethylamino-
carbonyl)-4-methylsulfonylbenzoate and 5 ml of thionyl
chloride was stirred for 6 hours at room temperature. The
10 solution was diluted with 50 ml of dichloromethane and
subsequently concentrated. The residue was dissolved in
20 ml of dichloromethane. The addition of cyclohexane
resulted in a crystalline precipitate which was filtered
off with suction and dried. This gave 6.4 g (88% of
theory) of methyl 2-chloro-3-(1'-chloro-2',2'-
15 dimethylethylaminocarbonyl)-4-methylsulfonylbenzoate.

Step e) 2-Chloro-3-(4',4'-dimethyl-4',5'-dihydroxazol-2-yl)-4-
methylsulfonylbenzoic acid (compound 4.38)

20 A solution of 5.82 g (15 mmol) of methyl
2-chloro-3-(1'-chloro-2',2'-dimethylethyl-
aminocarbonyl)-4-methylsulfonylbenzoate and 0.81 g
(20 mmol) of sodium hydroxide in 80 ml of methanol was
25 stirred for 8 hours at room temperature. After the solvent
had been distilled off, the residue was taken up in water
and the mixture was washed three times with ethyl
acetate. The aqueous phase was acidified with
hydrochloric acid and extracted three times with ethyl
30 acetate. After the organic phase had been dried, the
solvent was removed in vacuo. This gave 3.10 g (56% of
theory) of 2-chloro-3-(4',4'-dimethyl-4',5'-
dihydroxazol-2-yl)-4-methylsulfonylbenzoic acid.
(¹H NMR (δ in ppm): 1.34 (s); 3.40 (s); 4.13 (s); 8.07
(s); 13.95 (s, br)).

35 Step f) 2-Chloro-3-(1'-chloro-2',2'-dimethylethylaminocarbonyl)-
4-methylsulfonylbenzoyl chloride.

40 A solution of 3.00 g (9 mmol) of 2-chloro-3-(4',4'-
dimethyl-4',5'-dihydroxazol-2-yl)-4-methylsulfonyl-
benzoic acid, 1.43 g of thionyl chloride and 1 drop of
dimethylformamide in 80 ml of dry toluene was refluxed
for 3 hours. After cooling, the solvent was distilled off
45 in vacuo. This gave 3.43 g (86% of theory) of
2-chloro-3-(1'-chloro-2',2'-dimethylethylaminocarbonyl)-
4-methylsulfonylbenzoyl chloride.

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Methyl 2-chloro-3-(1,3,4-oxathiazolin-2-on-5-yl)-4-methylsulfonylbenzoate (compound 4.22)

5 Step a) Methyl 3-aminocarbonyl-2-chloro-4-methylsulfonylbenzoate

10 Ammonia was passed for 2 hours into a solution of 15.0 g (48 mmol) of methyl 2-chloro-3-chlorocarbonyl-4-methylsulfonylbenzoate and 300 ml of dry dioxane. The precipitate formed was filtered off with suction and the filtrate was concentrated. This gave 15.2 g of methyl 3-aminocarbonyl-2-chloro-4-methylsulfonylbenzoate in quantitative yield.

15 Step b) Methyl 2-chloro-3-(1,3,4-oxathiazolin-2-on-5-yl)-4-methylsulfonylbenzoate

20 9.80 g (75 mmol) of chlorocarbonylsulphenyl chloride were added dropwise to a solution of 4.37 g (15 mmol) of methyl 3-aminocarbonyl-2-chloro-4-methylsulfonylbenzoate in 150 ml of dry toluene. After the mixture had been stirred for 48 hours under reflux, the solvent was removed in vacuo and the residue was chromatographed on silica gel (eluent: ethyl acetate/cyclohexane = 1/1).
25 This gave 3.70 g (70% of theory) of methyl 2-chloro-3-(1,3,4-oxathiazolin-2-on-5-yl)-4-methylsulfonylbenzoate.

Methyl 2-chloro-4-methylsulfonyl-3-(4,5-dihydrooxazol-3-yl)-benzoate (compound 4.41)

30 At room temperature, 41.8 g (0.41 mol) of triethylamine and then 31.1 g (0.10 mol) of methyl 2-chloro-3-chlorocarbonyl-4-methylsulfonylbenzoate in 150 ml of toluene were added dropwise to 26.6 g (0.13 mol) of 1-amino-2-bromoethane hydrobromide in
35 500 ml of toluene. The mixture was heated under reflux for 5 hours and then stirred at room temperature for 12 hours, another 5.0 g (0.02 mol) of 1-amino-2-bromoethane hydrobromide were added and the mixture was heated under reflux for 7.5 hours. The reaction mixture was allowed to cool, diluted with ethyl
40 acetate, washed with water, dried and concentrated. The residue was then recrystallized from methyl tert-butyl ether/ethyl acetate. 14.5 g (46% of theory) of methyl 2-chloro-4-methylsulfonyl-3-(4,5-dihydrooxazol-2-yl)benzoate were obtained.

45 2-Chloro-3-(5-methoxy-5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid (compound 4.60)

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Step a) Methyl 2-chloro-3-(5-methoxy-5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate

5 7.3 g (102 mmol) of 2-methoxy-1-propene, 28 ml of sodium hypochlorite solution (12.5% strength) and a spatula-tip of sodium acetate were added successively to 10.0 g (34 mmol) of methyl 2-chloro-3-(hydroxyiminomethyl)-4-methylsulfonylbenzoate in 200 ml of methylene chloride. The mixture was stirred at room temperature for 12 hours, 10 the solvent was removed and the residue was taken up in ethyl acetate, washed with water, dried and concentrated. The residue was chromatographed over silica gel (eluent: cyclohexane:ethyl acetate = 3:2). This gave 5.8 g (47% of theory) of methyl 2-chloro-3-(5-methoxy-5-methyl-15 4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate. (mp.: 100-105°C)

Step b) 2-Chloro-3-(5-methoxy-5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate

20 At reflux temperature, 5.5 g (15.0 mmol) of methyl 2-chloro-3-(5-methoxy-5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate in 100 ml of pyridine were added dropwise to 5.0 g (37.5 mmol) of lithium iodide in 200 ml 25 of pyridine. The mixture was stirred at this temperature for 4 hours and then cooled, the solvent was distilled off and the residue was taken up in toluene and reconcentrated. The residue was subsequently admixed with water and washed with methylene chloride, and the pH was 30 adjusted to 1 using hydrochloric acid. The aqueous phase was extracted with methylene chloride and the resulting organic phase was dried and concentrated. This gave 4.7 g (90% of theory) of 2-chloro-(5-methoxy-5-methyl-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate. 35 (mp.: 40-45°C)

Methyl 2-chloro-3-(2-methyl-2H-1,3,4-dioxazol-5-yl)-4-methylsulfonylbenzoate (compound 4.44)

40 8.0 g (27.4 mmol) of methyl 2-chloro-3-(hydroxyiminomethyl)-4-methylsulfonylbenzoate in 150 ml of methylene chloride were admixed dropwise with 16.0 g (27.4 mmol) of a 12.5% strength sodium hypochlorite solution, and a spatula-tip of sodium acetate was added. After 1 hour, 34.4 g (0.74 mol) of acetaldehyde were 45 added a little at a time within a period of 36 hours, and the mixture was slowly heated to 55°C. The mixture was subsequently stirred at room temperature for 48 hours, washed with water,

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dried and concentrated. The residue was then taken up in methylene chloride, 10.0 g (0.23 mol) of acetaldehyde and a spatula-tip of sodium acetate were added and the mixture was heated under reflux for 8 hours. After 72 hours, a further 10.0 g
5 (0.23 mol) of acetaldehyde were added and the mixture was stirred at room temperature. The mixture was subsequently washed with water, dried and concentrated. The residue was passed through silica gel (eluent: isopropanol:cyclohexane = 1:9). This gave 5.0 g (55% of theory) of methyl 2-chloro-3-(2-methyl-
10 2H-1,3,4-dioxazol-5-yl)-4-methylsulfonylbenzoate.

Table 4 which follows lists the compounds which have been described above and also further benzoic acid derivatives of the formula III which were prepared, or can be prepared, by a similar
15 method.

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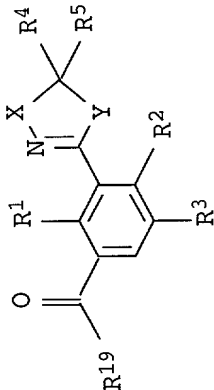
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Table 4:



III

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
4.1	Cl	Cl	H	O	H	H	CH ₂	OCH ₃	3.29 (t); 3.91 (s); 4.58 (t); 7.46 (d); 7.83 (d).
4.2	Cl	Cl	H	O	H	H	CH ₂	OH	3.28 (t); 4.60 (t); 7.02 (s, br); 7.46 (d); 7.98 (d).
4.3	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	OCH ₃	3.24 (s); 3.42 (t); 3.99 (s); 4.60 (t); 7.96 (d); 8.10 (d).
4.4	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	OH	3.26 (s); 3.45 (t); 4.63 (t); 8.15 (s); 8.53 (s, br).
4.5	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	Cl	3.25 (s); 3.46 (t); 4.62 (t); 8.21 (dd).
4.6	Cl	Cl	H	C(CH ₃) ₂	H	H	O	OH	1.31 (s); 4.16 (s); 7.69 (d); 7.90 (d); 13.8 (s, br).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
4.7	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	CH ₃	CH ₂	OCH ₃	1.25 (t); 1.57 (s); 3.21 (s); 3.42 (q); 3.99 (s); 7.94 (d); 8.07 (d).
4.8	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	CH ₃	CH ₂	OH	1.13 (t); 1.47 (s); 3.15 (s); 3.43 (q); 8.06 (s); 13.8 (s, br).
4.9	Cl	SO ₂ C ₂ H ₅	H	O	H	H	CH ₂	OCH ₃	1.28 (t); 3.41 (m); 4.02 (s); 4.62 (t); 7.95 (d); 8.06 (d).
4.10	Cl	SO ₂ C ₂ H ₅	H	O	H	H	CH ₂	OH	137-140
4.11	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	H	CH ₂	OCH ₃	1.26 (t); 1.53 (d); 3.06 (dd); 3.42 (q); 3.49 (dd); 5.05 (m); 7.95 (d); 8.07 (d).
4.12	Cl	SO ₂ C ₂ H ₅	H	O	CH ₃	H	CH ₂	OH	140-143
4.13	Cl	SO ₂ CH ₃	H	CH ₂	H	H	O	OCH ₃	3.30 (s); 3.98 (s); 4.11 (t); 4.55 (t); 7.97 (d); 8.08 (d).
4.14	Cl	SO ₂ CH ₃	H	CH ₂	H	H	O	OH	3.38 (s); 4.00 (t); 4.46 (t); 8.08 (s).
4.15	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	OH	3.30 (s); 3.35 (t); 4.15 (s, br); 4.50 (t); 8.05 (s).
4.16	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	CH ₃	CH ₂	OCH ₃	0.95 (t); 1.47 (s); 1.58 (quin); 3.12 (s); 3.31 (s); 3.43 (t); 3.93 (s); 8.09 (dd).
4.17	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	CH ₃	CH ₂	OH	0.93 (t); 1.47 (s); 1.58 (quin); 3.15 (s); 3.42 (t); 8.05 (s).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
4.18	Cl	SO ₂ -n-C ₃ H ₇	H	O	H	H	CH ₂	OCH ₃	0.92 (t); 1.55 (quin); 3.39 (m); 3.93 (s); 4.50 (t); 8.08 (dd).
4.19	Cl	SO ₂ -n-C ₃ H ₇	H	O	H	H	CH ₂	OH	148-150
4.20	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	H	CH ₂	OCH ₃	0.93 (t); 1.49 (d); 1.58 (quin); 2.94 (dd); 3.42 (m); 3.93 (s); 4.97 (m); 8.10 (dd).
4.21	Cl	SO ₂ -n-C ₃ H ₇	H	O	CH ₃	H	CH ₂	OH	0.94 (t); 1.39 (d); 1.58 (quin); 2.96 (dd); 3.50 (m); 4.95 (m); 8.05 (s).
4.22	Cl	SO ₂ CH ₃	H	S	=O		O	OCH ₃	3.24 (s); 4.02 (s); 8.14 (dd).
4.23	Cl	SO ₂ CH ₃	H	O	COOC ₂ H ₅	H	CH ₂	OCH ₃	118-121
4.24	Cl	SO ₂ CH ₃	H	O	COOC ₂ H ₅	H	CH ₂	OH	
4.25	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	OCH ₃	130-135
4.26	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	OH	173-178
4.27	Cl	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	OCH ₃	1.57 (s); 3.18 (s); 3.27 (s); 4.01 (s); 7.97 (d); 8.12 (d).
4.28	Cl	SO ₂ CH ₃	H	O	CH ₃	CH ₃	CH ₂	OH	1.48 (s); 3.15 (s); 3.34 (s); 8.08 (dd).
4.29	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	H	CH ₂	OCH ₃	0.97 (t); 1.72 (m); 3.10 (dd); 3.32 (s); 3.37 (dd); 4.72 (m); 8.08 (dd).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical data m.p. [°C]; ¹ H NMR [δ in ppm]
4.30	Cl	SO ₂ CH ₃	H	O	H	-(CH ₂) ₃ -CH-		OCH ₃	1.57 (m); 1.81 (m); 2.21 (m); 3.20 (s); 4.02 (s); 4.32 (t); 5.35 (dd); 7.92 (d); 8.18 (d).
4.31	Cl	SO ₂ CH ₃	H	O	H	-(CH ₂) ₃ -CH-		OH	1.72 (m); 2.01 (m); 3.27 (s); 4.24 (t); 5.23 (dd); 8.05 (d); 8.15 (d); 13.8 (s, br).
4.32	Cl	SO ₂ CH ₃	H	O	-(CH ₂) ₂ -O-(CH ₂) ₂ -		CH ₂	OCH ₃	2.00 (m); 3.23 (s); 3.27 (s), 3.72 (m); 4.00 (s); 7.96 (d); 8.04 (d).
4.33	Cl	SO ₂ CH ₃	H	O	-(CH ₂) ₂ -O-(CH ₂) ₂ -		CH ₂	OH	78-83
4.34	Cl	SO ₂ CH ₃	H	O	-(CH ₂) ₄ -		CH ₂	OCH ₃	1.78 (m); 2.24 (m); 3.27 (s); 3.36 (s); 3.98 (s); 7.94 (d); 8.12 (d).
4.35	Cl	SO ₂ CH ₃	H	O	-(CH ₂) ₄ -		CH ₂	OH	1.76 (m); 2.05 (m); 3.30 (s); 3.33 (s); 8.09 (dd).
4.36	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	C ₂ H ₅	CH ₂	OCH ₃	1.00 (t); 1.85 (m); 3.13 (s); 3.27 (s); 3.98 (s); 7.94 (d); 8.11 (d).
4.37	Cl	SO ₂ CH ₃	H	O	C ₂ H ₅	C ₂ H ₅	CH ₂	OH	0.91 (t); 1.76 (m); 3.12 (s); 3.33 (s); 8.07 (dd); 13.75 (s, br).
4.38	Cl	SO ₂ CH ₃	H	C(CH ₃) ₂	H	H	O	OH	1.34 (s); 3.40 (s); 4.13 (s); 8.07 (s); 13.95 (s, br).
4.39	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CH ₂	Cl	

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical Data m.p. [°C]; ¹ H-NMR [δ in ppm]
4.40	Cl	SO ₂ CH ₃	H	CH ₂	H	H	O	OH	> 260
4.41	Cl	SO ₂ CH ₃	H	CH ₂	H	H	O	OCH ₃	3.29 (3H); 3.96 (3H); 4.12 (2H); 4.55 (2H); 7.98 (1H); 8.09 (1H).
4.42	Cl	SCH ₃	H	O	H	H	CH ₂	OCH ₃	202-203
4.43	Cl	SO ₂ CH ₃	H	O	COOMe	H	CHCO ₂ CH ₃	OCH ₃	1.05 (3H); 1.35 (3H); 3.19 (3H); 4.01 (3H); 4.09 (2H); 4.35 (2H); 5.06 (1H); 5.77 (1H); 8.08 (1H); 8.17 (1H).
4.44	Cl	SO ₂ CH ₃	H	O	CH ₃	H	O	OCH ₃	1.78 (3H); 3.30 (3H); 3.98 (3H); 6.40 (1H); 8.08 (1H); 8.15 (1H).
4.45	Cl	SO ₂ CH ₃	H	O	CHO	H	CHCH ₃	OCH ₃	80-85
4.46	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₂ Cl	OCH ₃	1.65 (3H); 3.27 (3H); 3.50 (2H); 4.00 (3H); 4.22 (1H); 4.88/5.08 (1H); 7.99 (1H); 8.12 (1H).
4.47	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₂ Cl	OH	100-105
4.48	Cl	SO ₂ CH ₃	H	O	CHO	H	CHCH ₃	OH	180-185
4.49	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	OCH ₃	1.30 (3H); 2.75 (2H); 3.25 (1H); 3.34 (3H); 3.78 (1H); 3.94 (3H); 6.22 (1H); 8.15 (2H).
4.50	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	OH	65-67
4.51	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	OCH ₃	1.01 (3H); 1.28 (3H); 3.33 (4H); 3.96 (3H); 4.98 (1H); 8.12 (1H); 8.20 (1H).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical Data m.p. [°C]; ¹ H-NMR [δ in ppm]
4.52	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	OH	68-75
4.53	Cl	SO ₂ CH ₃	H	O	OCOCH ₃	H	CH ₂	OCH ₃	105-110
4.54	Cl	SO ₂ CH ₃	H	O	H	H	CH ₂	OH	
4.55	Cl	SO ₂ CH ₃	H	O	OCOCH ₃	H	CH ₂	OH	45-50
4.56	Cl	SO ₂ CH ₃	H	O	OCH ₃	H	CH ₂	OH	60-65
4.57	Cl	SO ₂ CH ₃	H	O	CHCl (CH ₃)	H	CH ₂	OCH ₃	1.63 (3H); 3.23 (3H); 3.50 (2H); 3.99 (3H); 4.25 (1H); 4.83/5.03 (1H); 7.96 (1H); 8.13 (1H).
4.58	Cl	SO ₂ CH ₃	H	O	CHCl (CH ₃)	H	CH ₂	OH	1.56 (3H); 3.33 (3H); 3.43 (2H); 4.36 (1H); 4.93 (1H); 8.10 (2H).
4.59	Cl	SO ₂ CH ₃	H	O	CH ₃	OCH ₃	CH ₂	OCH ₃	100-105
4.60	Cl	SO ₂ CH ₃	H	O	CH ₃	OCH ₃	CH ₂	OH	40-45
4.61	Cl	SO ₂ CH ₃	H	O	CF ₃	OCOCH ₃	CH ₂	OCH ₃	60-65
4.62	Cl	SCH ₃	H	O	H	H	CH ₂	OH	
4.63	Cl	SO ₂ Me	H	O	COCH ₃	H	CH ₂	OCH ₃	2.36 (3H); 3.25 (3H); 3.66 (2H); 4.01 (3H); 5.20 (1H); 8.01 (1H); 8.12 (1H).
4.64	Cl	SO ₂ CH ₃	H	O	CF ₃	H	CH ₂	OCH ₃	156
4.65	Cl	SO ₂ CH ₃	H	O	CF ₃	H	CH ₂	OH	170
4.66	Cl	SO ₂ CH ₃	H	O	F	F	CH ₂	OCH ₃	
4.67	Cl	SO ₂ CH ₃	H	O	F	F	CH ₂	OH	
4.68	Cl	SO ₂ CH ₃	H	O	F	H	CH ₂	OCH ₃	142-143

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical Data m.p. [°C]; ¹ H-NMR [δ in ppm]
4.69	Cl	SO ₂ CH ₃	H	O	F	H	CH ₂	OH	
4.70	Cl	SO ₂ CH ₃	H	O	CH ₂ Cl	H	CH ₂	OCH ₃	107-110
4.71	Cl	SO ₂ CH ₃	H	O	CH ₂ Cl	H	CH ₂	OH	60-65
4.72	Cl	SO ₂ CH ₃	H	O	OCH ₃	H	CH ₂	OCH ₃	105-110
4.73	Cl	SO ₂ CH ₃	H	O	OC ₂ H ₅	H	CH ₂	OCH ₃	155-160
4.74	Cl	SO ₂ CH ₃	H	CH ₂	H	H	S	OCH ₃	
4.75	CH ₃	H	H	C=O	H	H	S	OCH ₃	112-120
4.76	Cl	SO ₂ CH ₃	H	O	CF ₃	OH	CH ₂	OH	3.38 (s); 3.56 (d); 3.79 (d); 8.16 (s); 8.67 (s, br).
4.77	Cl	SO ₂ CH ₃	H	O	O-t-C ₄ H ₉	H	CH ₂	OCH ₃	130-135
4.78	Cl	SO ₂ CH ₃	H	O	O-t-C ₄ H ₉	H	CH ₂	OH	1.25 (s); 3.05 (dd); 3.34 (s); 3.45 (dd); 6.17 (m); 8.08 (s).
4.79	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	OCH ₃	1.01 (d); 1.28 (d); 3.35 (m); 3.96 (s); 4.99 (m); 8.12 (d); 8.20 (d).
4.80	Cl	SO ₂ CH ₃	H	O	CH ₃	H	CHCH ₃	OH	68-75
4.81	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	OCH ₃	1.30 (t); 2.77 (q); 3.25 (dd); 3.34 (s); 3.78 (dd); 3.94 (s); 6.22 (m), 8.24 (s).
4.82	Cl	SO ₂ CH ₃	H	O	SC ₂ H ₅	H	CH ₂	OH	65-67
4.83	SCH ₃	SCH ₃	H	O	H	H	CH ₂	OCH ₂ CH ₃	1.28 (t); 2.30 (s); 2.46 (s); 3.28 (t); 4.31 (q); 4.45 (t); 7.42 (d); 7.68 (d).

No.	R ¹	R ²	R ³	X	R ⁴	R ⁵	Y	R ¹⁹	Physical Data m.p. [°C]; ¹ H-NMR [δ in ppm]
4.84	SCH ₃	SCH ₃	H	O	H	H	CH ₂	OH	2.32 (s); 2.48 (s); 3.28 (t); 4.42 (t); 7.48 (d); 7.64 (d); 13.2 (s).
4.85	SO ₂ CH ₃	SO ₂ CH ₃	H	O	H	H	CH ₂	OH	3.25 (s); 3.35 (s); 3.44 (t); 8.05 (d); 8.45 (d).

The 3-heterocyclyl-substituted benzoyl derivatives of the formula I and their agriculturally useful salts are suitable as herbicides, both in the form of isomer mixtures and in the form of the pure isomers. The herbicidal compositions comprising compounds of the formula I effect very good control of vegetation on non-crop areas, especially at high rates of application. In crops such as wheat, rice, maize, soybeans and cotton they act against broad-leaved weeds and grass weeds without damaging the crop plants substantially. This effect is observed especially at low rates of application.

Depending on the application method in question, the compounds of the formula I, or herbicidal compositions comprising them, can additionally be employed in a further number of crop plants for eliminating undesirable plants. Examples of suitable crops are the following:

Allium cepa, Ananas comosus, Arachis hypogaea, Asparagus officinalis, Beta vulgaris spec. altissima, Beta vulgaris spec. rapa, Brassica napus var. napus, Brassica napus var. napobrassica, Brassica rapa var. silvestris, Camellia sinensis, Carthamus tinctorius, Carya illinoensis, Citrus limon, Citrus sinensis, Coffea arabica (Coffea canephora, Coffea liberica), Cucumis sativus, Cynodon dactylon, Daucus carota, Elaeis guineensis, Fragaria vesca, Glycine max, Gossypium hirsutum, (Gossypium arboreum, Gossypium herbaceum, Gossypium vitifolium), Helianthus annuus, Hevea brasiliensis, Hordeum vulgare, Humulus lupulus, Ipomoea batatas, Juglans regia, Lens culinaris, Linum usitatissimum, Lycopersicon lycopersicum, Malus spec., Manihot esculenta, Medicago sativa, Musa spec., Nicotiana tabacum (N.rustica), Olea europaea, Oryza sativa, Phaseolus lunatus, Phaseolus vulgaris, Picea abies, Pinus spec., Pisum sativum, Prunus avium, Prunus persica, Pyrus communis, Ribes sylvestre, Ricinus communis, Saccharum officinarum, Secale cereale, Solanum tuberosum, Sorghum bicolor (s. vulgare), Theobroma cacao, Trifolium pratense, Triticum aestivum, Triticum durum, Vicia faba, Vitis vinifera and Zea mays.

Moreover, the compounds of the formula I can also be used in crops which tolerate the action of herbicides due to breeding including genetic engineering methods.

The compounds of the formula I, or the herbicidal compositions comprising them, can be employed, for example, in the form of directly sprayable aqueous solutions, powders, suspensions, also

highly-concentrated aqueous, oily or other suspensions or dispersions, emulsions, oil dispersions, pastes, dusts, materials for spreading or granules, by means of spraying, atomizing, dusting, spreading or pouring. The use forms depend on the intended purposes; in any case, they should guarantee the finest possible distribution of the active ingredients according to the invention.

The herbicidal compositions comprise a herbicidally active amount of at least one compound of the formula I or of an agriculturally useful salt of I and auxiliaries conventionally used for the formulation of crop protection products.

Suitable inert auxiliaries are essentially:

mineral oil fractions of medium to high boiling point such as kerosene and diesel oil, furthermore coal tar oils and oils of vegetable or animal origin, aliphatic, cyclic and aromatic hydrocarbons, eg. paraffins, tetrahydronaphthalene, alkylated naphthalenes and their derivatives, alkylated benzenes and their derivatives, alcohols such as methanol, ethanol, propanol, butanol and cyclohexanol, ketones such as cyclohexanone, strongly polar solvents, eg. amines such as N-methylpyrrolidone and water.

Aqueous use forms can be prepared from emulsion concentrates, suspensions, pastes, wettable powders or water-dispersible granules by adding water. To prepare emulsions, pastes or oil dispersions, the substances, as such or dissolved in an oil or solvent, can be homogenized in water by means of wetting agent, tackifier, dispersant or emulsifier. However, it is also possible to prepare concentrates composed of active substance, wetting agent, tackifier, dispersant or emulsifier and, if appropriate, solvent or oil, and these concentrates are suitable for dilution with water.

Suitable surfactants (adjuvants) are the alkali metal, alkaline earth metal and ammonium salts of aromatic sulfonic acids, eg. ligno-, phenol-, naphthalene- and dibutylnaphthalenesulfonic acid, and of fatty acids, of alkyl- and alkylaryl sulfonates, of alkyl sulfates, lauryl ether sulfates and fatty alcohol sulfates, and salts of sulfated hexa-, hepta- and octadecanols, and of fatty alcohol glycol ether, condensates of sulfonated naphthalene and its derivatives with formaldehyde, condensates of naphthalene, or of the naphthalenesulfonic acids, with phenol and formaldehyde, polyoxyethylene octylphenyl ether, ethoxylated isooctyl-, octyl- or nonylphenol, alkylphenyl, tributylphenyl polyglycol ether, alkylaryl polyether alcohols, isotridecyl

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alcohol, fatty alcohol ethylene oxide condensates, ethoxylated castor oil, polyoxyethylene alkyl ethers or polyoxypropylene alkyl ethers, lauryl alcohol polyglycol ether acetate, sorbitol esters, lignin-sulfite waste liquors or methylcellulose.

5

Powders, materials for spreading and dusts can be prepared by mixing or concomitantly grinding the active substances with a solid carrier.

10

Granules, eg. coated granules, impregnated granules and homogeneous granules, can be prepared by binding the active ingredients to solid carriers. Solid carriers are mineral earths such as silicas, silica gels, silicates, talc, kaolin, limestone,

15

lime, chalk, bolus, loess, clay, dolomite, diatomaceous earth, calcium sulfate, magnesium sulfate, magnesium oxide, ground synthetic material, fertilizers such as ammonium sulfate, ammonium phosphate, ammonium nitrate, ureas and products of vegetable origin such as cereal meal, tree bark meal, wood meal and nutshell meal, cellulose powders or other solid carriers.

20

The concentrations of the compounds of the formula I in the ready-to-use products can be varied within wide ranges. In general, the formulations comprise approximately from 0.001 to 98% by weight, preferably 0.01 to 95% by weight, of at least one active ingredient. The active ingredients are employed in a purity of from 90% to 100%, preferably 95% to 100% (according to NMR spectrum).

25

30 The formulation examples below illustrate the preparation of such products:

I. 20 parts by weight of the compound No. 3.2 are dissolved in a mixture composed of 80 parts by weight of alkylated benzene, 10 parts by weight of the adduct of 8 to 10 mol of ethylene oxide and 1 mol of oleic acid N-monoethanolamide, 5 parts by weight of calcium dodecylbenzenesulfonate and 5 parts by weight of the adduct of 40 mol of ethylene oxide and 1 mol of castor oil. Pouring the solution into 100,000 parts by weight of water and finely distributing it therein gives an aqueous dispersion which comprises 0.02% by weight of the active ingredient.

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II. 20 parts by weight of the compound No. 3.9 are dissolved in a mixture composed of 40 parts by weight of cyclohexanone, 30 parts by weight of isobutanol, 20 parts by weight of the adduct of 7 mol of ethylene oxide and 1 mol of

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- isooctylphenol and 10 parts by weight of the adduct of 40 mol of ethylene oxide and 1 mol of castor oil. Pouring the solution into 100,000 parts by weight of water and finely distributing it therein gives an aqueous dispersion which comprises 0.02% by weight of the active ingredient.
- 5
- III. 20 parts by weight of the active ingredient No. 3.10 are dissolved in a mixture composed of 25 parts by weight of cyclohexanone, 65 parts by weight of a mineral oil fraction of boiling point 210 to 280°C and 10 parts by weight of the adduct of 40 mol of ethylene oxide and 1 mol of castor oil. Pouring the solution into 100,000 parts by weight of water and finely distributing it therein gives an aqueous dispersion which comprises 0.02% by weight of the active ingredient.
- 10
- 15
- IV. 20 parts by weight of the active ingredient No. 3.16 are mixed thoroughly with 3 parts by weight of sodium diisobutyl-naphthalenesulfonate, 17 parts by weight of the sodium salt of a lignosulfonic acid from a sulfite waste liquor and 60 parts by weight of pulverulent silica gel and the mixture is ground in a hammer mill. Finely distributing the mixture in 20,000 parts by weight of water gives a spray mixture which comprises 0.1% by weight of the active ingredient.
- 20
- 25
- V. 3 parts by weight of the active ingredient No. 3.21 are mixed with 97 parts by weight of finely divided kaolin. This gives a dust which comprises 3% by weight of the active ingredient.
- 30
- VI. 20 parts by weight of the active ingredient No. 3.22 are mixed intimately with 2 parts by weight of calcium dodecylbenzenesulfonate, 8 parts by weight of fatty alcohol polyglycol ether, 2 parts by weight of the sodium salt of a phenol/urea/formaldehyde condensate and 68 parts by weight of a paraffinic mineral oil. This gives a stable oily dispersion.
- 35
- 40
- VII. 1 part by weight of the active ingredient No. 3.34 is dissolved in a mixture composed of 70 parts by weight of cyclohexanone, 20 parts by weight of ethoxylated isooctylphenol and 10 parts by weight of ethoxylated castor oil. This gives a stable emulsion concentrate.
- 45

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VIII. 1 part by weight of active ingredient No. 3.35 is dissolved in a mixture composed of 80 parts by weight of cyclohexanone and 20 parts by weight of Wettol[®] EM 31 (= nonionic emulsifier based on ethoxylated castor oil).

5 This gives a stable emulsion concentrate.

The compounds of the formula I, or the herbicidal compositions comprising them, can be applied pre- or post-emergence. If the active ingredients are less well tolerated by certain crop
10 plants, application techniques may be used in which the herbicidal compositions are sprayed, with the aid of the spray apparatus, in such a way that they come into as little contact as possible, if any, with the leaves of the sensitive crop plants while reaching the leaves of undesirable plants which grow
15 underneath, or the bare soil (post-directed, lay-by).

Depending on the intended aim of the control measures, the season, the target plants and the growth stage, the application
20 rates of the compound of the formula I are from 0.001 to 3.0, preferably 0.01 to 1.0 kg/ha of active substanz (a.s.).

To widen the spectrum of action and to achieve synergistic effects, the 3-heterocyclyl-substituted benzoyl derivatives of
25 the formula I can be mixed and applied jointly with a large number of representatives of other groups of herbicidally or growth-regulatory active ingredients. Suitable components in mixtures are, for example, 1,2,4-thiadiazoles, 1,3,4-thiadiazoles, amides, aminophosphoric acid and its
30 derivatives, aminotriazoles, anilides, aryloxy-/hetaryloxyalkanic acids and their derivatives, benzoic acid and its derivatives, benzothiadiazinones, 2-(hetaroyl/aroyl)-1,3-cyclohexandiones, hetaryl aryl ketones, benzylisoxazolidinones, meta-CF₃-phenyl derivatives, carbamates, quinolinecarboxylic acid and its
35 derivatives, chloroacetanilides, cyclohexenone oxime ether derivatives, diazines, dichloropropionic acid and its derivatives, dihydrobenzofuranes, dihydrofuran-3-ones, dinitroanilines, dinitrophenols, diphenyl ethers, dipyridyls, halocarboxylic acids and their derivatives, ureas,
40 3-phenyluracils, imidazoles, imidazolinones, N-phenyl-3,4,5,6-tetrahydrophthalimides, oxadiazoles, oxiranes, phenols, aryloxy- and hetaryloxyphenoxypionic esters, phenylacetic acid and its derivatives, 2-phenylpropionic acid and its derivatives, pyrazoles, phenylpyrazoles, pyridazines,
45 pyridinecarboxylic acid and its derivatives, pyrimidyl ethers,

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sulfonamides, sulfonylureas, triazines, triazinones, triazolinones, triazolcarboxamides and uracils.

- Moreover, it may be advantageous to apply the compounds of the formula I, alone or in combination with other herbicides, in the form of a mixture with additional other crop protection agents, for example with pesticides or agents for controlling phytopathogenic fungi or bacteria. Also of interest is the miscibility with mineral salt solutions which are employed for treating nutritional and trace element deficiencies. Non-phytotoxic oils and oil concentrates can also be added.

Use Examples

- The herbicidal action of 3-heterocyclyl-substituted benzoyl derivatives of the formula I was demonstrated by the following greenhouse experiments:
- The culture containers used were plastic flowerpots containing loamy sand with approximately 3.0% of humus as substrate. The seeds of the test plants were sown separately for each species.
- For the pre-emergence treatment, the active ingredients, suspended or emulsified in water, were applied directly after sowing by means of finely distributing nozzles. The containers were irrigated gently to promote germination and growth and subsequently covered with transparent plastic hoods until the plants had rooted. This cover caused uniform germination of the test plants unless this was adversely affected by the active ingredients.
- For the post-emergence treatment, the test plants were grown to a plant height of from 3 to 15 cm, depending on the plant habit, and only then treated with the active ingredients which had been suspended or emulsified in water. To this end, the test plants were either sown directly and grown in the same containers, or they were first grown separately as seedlings and transplanted into the test containers a few days prior to treatment. The rate of application for the post-emergence treatment was 31.2 or 15.6 g/ha a.s. (active substance).

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Depending on the species, the plants were kept at from 10 to 25°C and 20 to 35°C, respectively. The test period extended over 2 to 4 weeks. During this time, the plants were tended, and their response to the individual treatments was evaluated.

5

Evaluation was carried out using a scale of from 0 to 100. 100 means no emergence of the plants, or complete destruction of at least the aerial parts, and 0 means no damage or normal course of growth.

10

The plants used in the greenhouse experiments belonged to the following species:

15	Scientific name	Common name
	Chenopodium album	lambsquarters (goosefoot)
	Setaria faberii	giant foxtail
	Sinapsis alba	white mustard
20	Solanum nigrum	black nightshade
	Triticum aestivum	wheat
	Zea mays	Indian corn

25 Compound 3.33 (Table 3) was very effective against the abovementioned mono- and dicotyledonous harmful plants and was well tolerated in winter wheat and maize when applied post-emergence at rates of application of 31.2 and 15.6 g/ha, respectively.

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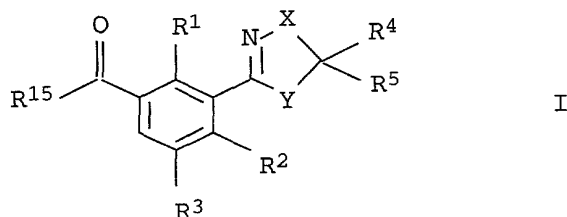
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We claim

1. A 3-heterocyclyl-substituted benzoyl derivative of the formula I



where the variables have the following meanings:

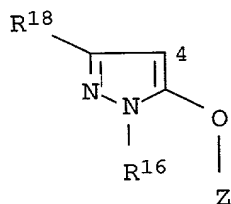
- R^1, R^2 are hydrogen, nitro, halogen, cyano, C_1 - C_6 -alkyl, C_1 - C_6 -haloalkyl, C_1 - C_6 -alkoxy, C_1 - C_6 -haloalkoxy, C_1 - C_6 -alkylthio, C_1 - C_6 -haloalkylthio, C_1 - C_6 -alkylsulfinyl, C_1 - C_6 -haloalkylsulfinyl, C_1 - C_6 -alkylsulfonyl or C_1 - C_6 -haloalkylsulfonyl;
- R^3 is hydrogen, halogen or C_1 - C_6 -alkyl;
- R^4, R^5 are hydrogen, halogen, cyano, nitro, C_1 - C_4 -alkyl, C_1 - C_4 -alkoxy- C_1 - C_4 -alkyl, di(C_1 - C_4 -alkoxy)- C_1 - C_4 -alkyl, di(C_1 - C_4 -alkyl)-amino- C_1 - C_4 -alkyl, [2,2-di(C_1 - C_4 -alkyl)-1-hydrazino]- C_1 - C_4 -alkyl, C_1 - C_6 -alkyliminoxy- C_1 - C_4 -alkyl, C_1 - C_4 -alkoxycarbonyl- C_1 - C_4 -alkyl, C_1 - C_4 -alkylthio- C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, C_1 - C_4 -cyanoalkyl, C_3 - C_8 -cycloalkyl, C_1 - C_4 -alkoxy, C_1 - C_4 -alkoxy- C_2 - C_4 -alkoxy, C_1 - C_4 -haloalkoxy, hydroxyl, C_1 - C_4 -alkylcarbonyloxy, C_1 - C_4 -alkylthio, C_1 - C_4 -haloalkylthio, di(C_1 - C_4 -alkyl)amino, COR⁶, phenyl or benzyl, it being possible for the two last-mentioned substituents to be fully or partially halogenated and/or to have attached to them one to three of the following groups:
nitro, cyano, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, C_1 - C_4 -alkoxy or C_1 - C_4 -haloalkoxy;

or

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R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be
 mono- to tetrasubstituted by C₁-C₄-alkyl and/or
 which can be interrupted by oxygen or by a
 nitrogen which is unsubstituted or substituted by
 C₁-C₄-alkyl;
 or
 R⁴ and R⁵ together with the corresponding carbon form a
 carbonyl or thiocarbonyl group;
 R⁶ is hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy,
 C₁-C₄-haloalkoxy, C₃-C₆-alkenyloxy, C₃-C₆-alkynyloxy
 or NR⁷R⁸;
 R⁷ is hydrogen or C₁-C₄-alkyl;
 R⁸ is C₁-C₄-alkyl;
 X is O, S, NR⁹, CO or CR¹⁰R¹¹;
 Y is O, S, NR¹², CO or CR¹³R¹⁴;
 R⁹, R¹² are hydrogen or C₁-C₄-alkyl;
 R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or
 CONR⁷R⁸;
 or
 R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together
 form a C₂-C₆-alkanediyl chain which can be mono- to
 tetrasubstituted by C₁-C₄-alkyl and/or interrupted
 by oxygen or by a nitrogen which is unsubstituted
 or substituted by C₁-C₄-alkyl;
 R¹⁵ is a pyrazole of the formula II which is linked in
 the 4-position

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II

where

R^{16} is C_1 - C_6 -alkyl;

Z is H or SO_2R^{17} ;

R^{17} is C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups: nitro, cyano, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl, C_1 - C_4 -alkoxy or C_1 - C_4 -haloalkoxy;

R^{18} is hydrogen or C_1 - C_6 -alkyl;

where X and Y are not simultaneously sulfur;

with the exception of

4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1-ethyl-5-hydroxy-1H-pyrazole,
 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
 4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and
 4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonyl-benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;

or an agriculturally useful salt thereof.

2. A 3-heterocycl-yl-substituted benzoyl derivative of the formula I where the variables have the following meanings:

R^1 , R^2 are hydrogen, nitro, halogen, cyano, C_1 - C_6 -alkyl, C_1 - C_6 -haloalkyl, C_1 - C_6 -alkoxy, C_1 - C_6 -haloalkoxy, C_1 - C_6 -alkylthio, C_1 - C_6 -haloalkylthio,

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C₁-C₆-alkylsulfinyl, C₁-C₆-haloalkylsulfinyl,
C₁-C₆-alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;

- 5 R³ is hydrogen, halogen or C₁-C₆-alkyl;
- 10 R⁴, R⁵ are hydrogen, halogen, cyano, nitro, C₁-C₄-alkyl,
C₁-C₄-alkoxy-C₁-C₄-alkyl, di(C₁-C₄-alkoxy)-C₁-C₄-
alkyl, di(C₁-C₄-alkyl)-amino-C₁-C₄-alkyl,
[2,2-di(C₁-C₄-alkyl)-1-hydrazino]-C₁-C₄-alkyl,
C₁-C₆-alkyliminoxy-C₁-C₄-alkyl, C₁-C₄-alkoxycarbonyl-
C₁-C₄-alkyl, C₁-C₄-alkylthio-C₁-C₄-alkyl,
C₁-C₄-haloalkyl, C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl,
C₁-C₄-alkoxy, C₁-C₄-alkoxy-C₂-C₄-alkoxy,
15 C₁-C₄-haloalkoxy, C₁-C₄-alkylthio,
C₁-C₄-haloalkylthio, di(C₁-C₄-alkyl)amino, COR⁶,
phenyl or benzyl, it being possible for the two
last-mentioned substituents to be fully or partially
halogenated and/or to have attached to them one to
20 three of the following groups:
nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;
- 25 or
- 30 R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be
mono- to tetrasubstituted by C₁-C₄-alkyl and/or
which can be interrupted by oxygen or by a
nitrogen which is unsubstituted or substituted by
C₁-C₄-alkyl;
- 35 or
- 40 R⁴ and R⁵ together with the corresponding carbon form a
carbonyl or thiocarbonyl group;
- 45 R⁶ is C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy,
C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy,
C₃-C₆-alkenyloxy, C₃-C₆-alkynyloxy or NR⁷R⁸;
- R⁷ is hydrogen or C₁-C₄-alkyl;
- R⁸ is C₁-C₄-alkyl;

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X is O, S, NR⁹, CO or CR¹⁰R¹¹;

Y is O, S, NR¹², CO or CR¹³R¹⁴;

5 R⁹, R¹² are hydrogen or C₁-C₄-alkyl;

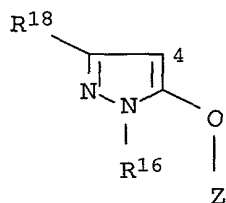
10 R¹⁰, R¹¹, R¹³, R¹⁴ are hydrogen, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxycarbonyl, C₁-C₄-haloalkoxycarbonyl or CONR⁷R⁸;

or

15 R⁴ and R⁹ or R⁴ and R¹⁰ or R⁵ and R¹² or R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

20 R¹⁵ is a pyrazole of the formula II which is linked in the 4-position

25



II

30

where

R¹⁶ is C₁-C₆-alkyl;

35

Z is H or SO₂R¹⁷;

40

R¹⁷ is C₁-C₄-alkyl, C₁-C₄-haloalkyl, phenyl or phenyl which is partially or fully halogenated and/or has attached to it one to three of the following groups: nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl, C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;

45

R¹⁸ is hydrogen or C₁-C₆-alkyl;

where X and Y are not simultaneously oxygen or sulfur;

with the exception of

- 5 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-
benzoyl]-1-ethyl-5-hydroxy-1H-pyrazole,
4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-
benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
4-[2-chloro-3-(5-cyano-4,5-dihydroisoxazol-3-yl)-4-methyl-
sulfonylbenzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole,
10 4-[2-chloro-3-(4,5-dihydrothiazol-2-yl)-4-methylsulfonyl-
benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole and
4-[2-chloro-3-(thiazoline-4,5-dion-2-yl)-4-methylsulfonyl-
benzoyl]-1,3-dimethyl-5-hydroxy-1H-pyrazole;
- 15 or an agriculturally useful salt thereof.
3. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in claim 1 or 2, where R³ is hydrogen.
- 20 4. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in any of claims 1 to 3, where
- 25 R¹, R² are nitro, halogen, cyano, C₁-C₆-alkyl,
C₁-C₆-haloalkyl, C₁-C₆-alkoxy, C₁-C₆-haloalkoxy,
C₁-C₆-alkylthio, C₁-C₆-haloalkylthio,
C₁-C₆-alkylsulfinyl, C₁-C₆-haloalkylsulfinyl,
C₁-C₆-alkylsulfonyl or C₁-C₆-haloalkylsulfonyl.
- 30 5. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in any of claims 1 to 4, where Z is
SO₂R¹⁷.
- 35 6. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in any of claims 1 to 4, where Z is
hydrogen.
- 40 7. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in any of claims 1 to 4 or 6, where X is
oxygen and Y is CR¹³R¹⁴.
- 45 8. A 3-heterocyclyl-substituted benzoyl derivative of the
formula I as claimed in any of claims 1 to 4 or 6 or 7, where

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- R⁴ is halogen, nitro, C₁-C₄-alkyl,
 C₁-C₄-alkoxy-C₁-C₄-alkyl,
 C₁-C₄-alkoxycarbonyl-C₁-C₄-alkyl,
 C₁-C₄-alkylthio-C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-cyanoalkyl, C₃-C₈-cycloalkyl, C₁-C₄-alkoxy,
 C₁-C₄-alkoxy-C₂-C₄-alkoxy, C₁-C₄-haloalkoxy,
 C₁-C₄-alkylthio, C₁-C₄-haloalkylthio,
 di(C₁-C₄-alkyl)amino, COR⁶, phenyl or benzyl, it
 being possible for the two last-mentioned
 substituents to be partially or fully halogenated
 and/or to have attached to them one to three of
 the following groups:
 nitro, cyano, C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-alkoxy or C₁-C₄-haloalkoxy;
- R⁵ is hydrogen or C₁-C₄-alkyl;
- or
- R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be
 mono- to tetrasubstituted by C₁-C₄-alkyl and/or
 which can be interrupted by oxygen or by a
 nitrogen which is unsubstituted or substituted by
 C₁-C₄-alkyl;
- or
- R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be
 mono- to tetrasubstituted by C₁-C₄-alkyl and/or
 which can be interrupted by oxygen or by a
 nitrogen which is unsubstituted or substituted by
 C₁-C₄-alkyl.
9. A 3-heterocyclyl-substituted benzoyl derivative of the
 formula I as claimed in any of claims 1 to 4 or 6 to 8, where
- R⁴ is C₁-C₄-alkyl, C₁-C₄-haloalkyl,
 C₁-C₄-alkoxycarbonyl or CONR⁷R⁸;
- R⁵ is hydrogen or C₁-C₄-alkyl;
- or

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R⁴ and R⁵ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl;

or

R⁵ and R¹³ together form a C₂-C₆-alkanediyl chain which can be mono- to tetrasubstituted by C₁-C₄-alkyl and/or which can be interrupted by oxygen or by a nitrogen which is unsubstituted or substituted by C₁-C₄-alkyl.

10. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 7, where R⁴ and R⁵ are hydrogen.

11. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 7 or 10, where R¹⁸ is hydrogen.

12. 4-[2-Chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonyl-benzoyl]-1-methyl-5-hydroxy-1H-pyrazole.

13. An agriculturally useful salt of 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-1-methyl-5-hydroxy-1H-pyrazole.

14. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6, where

X is S, NR⁹, CO or CR¹⁰R¹¹;

or

Y is O, S, NR¹² or CO.

15. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 14, where R¹⁸ is hydrogen.

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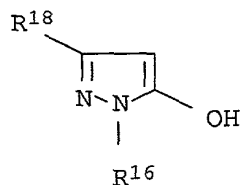
16. A 3-heterocyclyl-substituted benzoyl derivative of the formula I as claimed in any of claims 1 to 4 or 6 or 14, where

- 5 R^4 is halogen, cyano, nitro, C_1 - C_4 -alkyl,
 C_1 - C_4 -alkoxy- C_1 - C_4 -alkyl,
 C_1 - C_4 -alkoxycarbonyl- C_1 - C_4 -alkyl,
 C_1 - C_4 -alkylthio- C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl,
 C_1 - C_4 -cyanoalkyl, C_3 - C_8 -cycloalkyl, C_1 - C_4 -alkoxy,
 10 C_1 - C_4 -alkoxy- C_2 - C_4 -alkoxy, C_1 - C_4 -haloalkoxy,
 C_1 - C_4 -alkylthio, C_1 - C_4 -haloalkylthio,
 di(C_1 - C_4 -alkyl)amino, COR⁶, phenyl or benzyl, it
 being possible for the two last-mentioned
 substituents to be partially or fully halogenated
 15 and/or to have attached to them one to three of
 the following groups:
 nitro, cyano, C_1 - C_4 -alkyl, C_1 - C_4 -haloalkyl,
 C_1 - C_4 -alkoxy or C_1 - C_4 -haloalkoxy;
- 20 R^5 is hydrogen or C_1 - C_4 -alkyl;
- or
- 25 R^4 and R^5 together form a C_2 - C_6 -alkanediyl chain which can be
 mono- to tetrasubstituted by C_1 - C_4 -alkyl and/or
 which can be interrupted by oxygen or by a
 nitrogen which is unsubstituted or substituted by
 C_1 - C_4 -alkyl;
- 30 or
- 35 R^4 and R^9 or R^4 and R^{10} or R^5 and R^{12} or R^5 and R^{13} together
 form a C_2 - C_6 -alkanediyl chain which can be mono- to
 tetrasubstituted by C_1 - C_4 -alkyl and/or which can be
 interrupted by oxygen or by a nitrogen which is
 unsubstituted or substituted by C_1 - C_4 -alkyl;
- 40 R^{18} is C_1 - C_6 -alkyl.

17. A process for the preparation of 3-heterocyclyl-substituted benzoyl derivatives of the formula I as claimed in claim 1, which comprises acylating the pyrazole of the formula II
 45 where Z = H, where the variables R^{16} and R^{18} have the meanings given under claim 1,

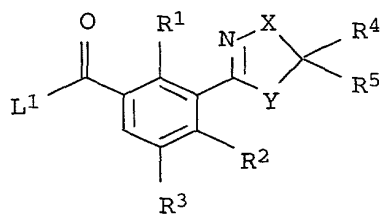
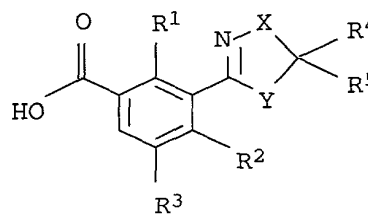
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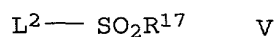


II (where Z = H)

with an activated carboxylic acid III α or with a carboxylic acid III β ,

III α III β

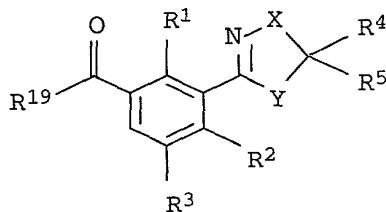
where the variables R¹ to R⁵, X and Y have the meanings given under claim 1 and L¹ is a nucleophilically displaceable leaving group, subjecting the acylation product to a rearrangement reaction in the presence or absence of a catalyst to give the compounds I (where Z = H) and, if desired, to prepare 3-heterocyclyl-substituted benzoyl derivatives of the formula I where Z = SO₂R¹⁷, reacting the product with a compound of the formula V,



where R¹⁷ has the meaning given under claim 1 and L² is a nucleophilically displaceable leaving group.

18. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III,

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III

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where R¹⁹ is hydroxyl or a radical which can be removed by hydrolysis and variables R¹ to R⁵, X and Y have the meanings given under the claims 1 to 16, with the exception of methyl 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoate, methyl 2-chloro-3-(4,5-dihydrooxazol-2-yl)-4-methylsulfonylbenzoate and methyl 2,4-dichloro-3-(5-methylcarbonyloxy-4,5-dihydroisoxazol-3-yl)benzoate.

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19. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III as claimed in claim 18 where the variables R¹ to R⁵, X and Y have the meanings given under claims 2 to 16.

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20. A 3-heterocyclyl-substituted benzoic acid derivative of the formula III as claimed in either of claims 18 or 19, where

R¹⁹ is halogen, hydroxyl or C₁-C₆-alkoxy.

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21. A composition comprising a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16, and auxiliaries conventionally used for the formulation of crop protection products.

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22. A process for the preparation of a composition as claimed in claim 21, which comprises mixing a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16 and auxiliaries conventionally used for the formulation of crop protection products.

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23. A method of controlling undesirable vegetation, which comprises allowing a herbicidally active amount of at least one 3-heterocyclyl-substituted benzoyl derivative of the

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formula I or of an agriculturally useful salt of I as claimed in any of claims 1 to 16 to act on plants, their environment and/or on seeds.

- 5 24. The use of a 3-heterocyclyl-substituted benzoyl derivative of the formula I or an agriculturally useful salt thereof as claimed in any of claims 1 to 16 as herbicide.

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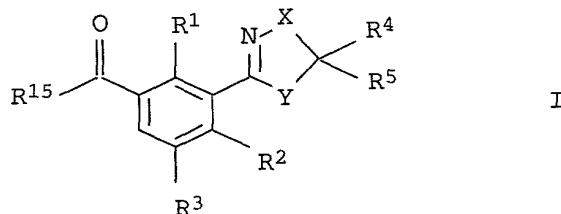
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P69T90 "0050/47679"

3-Heterocyclyl-substituted benzoyl derivatives

5 Abstract

Benzoyl derivatives of the formula I



where the variables have the following meanings:

- 20 R¹, R² are hydrogen, nitro, halogen, cyano, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl or C₁-C₆-haloalkylsulfonyl;
- 25 R³ is hydrogen, halogen or alkyl;
- R⁴, R⁵ are hydrogen, halogen, cyano, nitro, alkyl, alkoxy, alkylthio, dialkylamino, phenyl or carbonyl, it being possible for the 6 last-mentioned radicals to be substituted;
- 30
- X is O, S, NR⁹, CO or CR¹⁰R¹¹;
- 35 Y is O, S, NR¹², CO or CR¹³R¹⁴;
- R¹⁵ is pyrazole which is unsubstituted or substituted, linked in the 4-position and has attached to it in the 5-position a hydroxyl or sulfonyloxy radical;
- 40

and the agriculturally useful salts thereof; processes and intermediates for the preparation of the 3-heterocycl-yl-substituted benzoyl derivatives; compositions comprising them; and the use of these derivatives or compositions comprising them for controlling undesirable plants.

Declaration, Power of Attorney

Page 1 of 6

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We (I), the undersigned inventor(s), hereby declare(s) that:

My residence, post office address and citizenship are as stated below next to my name,

We (I) believe that we are (I am) the original, first, and joint (sole) inventor(s) of the subject matter which is claimed and for which a patent is sought on the invention entitled

3-Heterocyclyl-substituted benzoyl derivatives

the specification of which

☒ is attached hereto.

☐ was filed on _____ as

Application Serial No. _____

and amended on _____.

☒ was filed as PCT international application

Number PCT/EP 98/00069

on 08/01/1998

and was amended under PCT Article 19

on _____ (if applicable).

We (I) hereby state that we (I) have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

We (I) acknowledge the duty to disclose information known to be material to the patentability of this application as defined in Section 1.56 of Title 37 Code of Federal Regulations.

We (I) hereby claim foreign priority benefits under 35 U.S.C. § 119(a)-(d) or § 365(b) of any foreign application(s) for patent or inventor's certificate, or § 365(a) of any PCT International application which designated at least one country other than the United States, listed below and have also identified below, by checking the box, any foreign application for patent or inventor's certificate, or PCT International application having a filing date before that of the application on which priority is claimed. Prior Foreign Application(s)

Application No.	Country	Day/Month/Year	Priority Claimed
19701446.1	Federal Republic of Germany	17th January 1997	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No

O. Z. 0050/47679

We (I) hereby claim the benefit under Title 35, United States Codes, § 119(e) of any United States provisional application(s) listed below.

 (Application Number)

 (Filing Date)

 (Application Number)

 (Filing Date)

We (I) hereby claim the benefit under 35 U.S.C. § 120 of any United States application(s), or § 365(c) of any PCT International application designating the United States, listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in the prior United States or PCT International application in the manner provided by the first paragraph of 35 U.S.C. § 112, I acknowledge the duty to disclose information which is material to patentability as defined in 37 CFR § 1.56 which became available between the filing date of the prior application and the national or PCT International filing date of this application.

Application Serial No.	Filing Date	Status (pending, patented, abandoned)
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<hr/>	<hr/>	<hr/>

And we (I) hereby appoint **Messrs. HERBERT B. KEIL**, Registration Number 18,967; and **RUSSEL E. WEINKAUF**, Registration Number 18,495; the address of both being Messrs. Keil & Weinkauf, 1101 Connecticut Ave., N.W., Washington, D.C. 20036 (telephone 202-659-0100), our attorneys, with full power of substitution and revocation, to prosecute this application, to make alterations and amendments therein, to sign the drawings, to receive the patent, and to transact all business in the Patent Office connected therewith.

We (I) declare that all statements made herein of our (my) own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issuing thereon.

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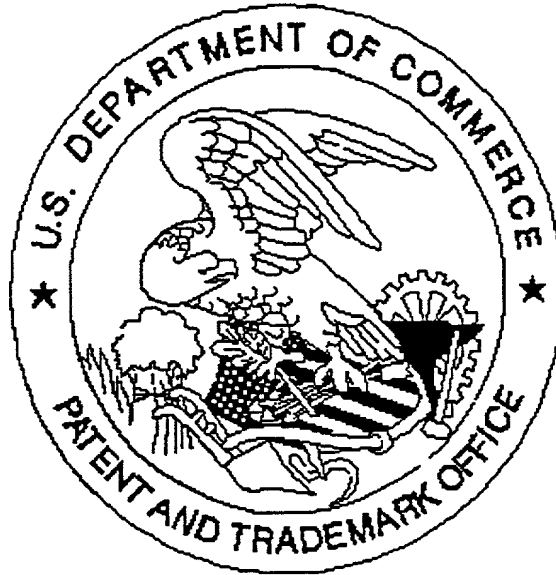
Joachim Rheinheimer

67063 Ludwigshafen ✓) ~~2~~ ✓

Joan Kleber

January 30, 1998

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